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Approximate Methods for the Optimal Control of Nonlinear Systems.

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APPROXIMATE METHODS FOR THE OPTIMAL CONTROL OF NONLINEAR SYSTEMS

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Abstract

Approximate and short-cut methods are developed in this dissertation for the optimal control of nonlinear systems. The chemical reactor, an important nonlinear system, is used as an example throughout this work. No experimental studies are carried out; all of the work is done on the XDS Sigma V digital computer, the IBM 360/65 digital computer and the XDS Sigma V - EAI 680 hybrid computer.

Two short-cut methods are developed that deal with the optimal temperature for homogenous, reversible, exothermic reactions.. The first consists of a series of graphs that allow the user to pick off the optimal temperature for isothermal operations of batch and plug flow reactors. The second is a simplified graphical method for the calculation of optimal temperature profiles.

An approximate, direct finite difference method is developed and applied to many linear and nonlinear optimal control problems. The results are compared with the optimal values.

A parameter search is used to determine, approximately, optimal closed loop algorithms for nonlinear systems. The results are compared with those obtained by linearization and the application of optimal control theory.

The problem of determining approximate optimal closed loop control for nonlinear systems was also approached from a more theoretical standpoint, based on the maximum principle. This study resulted in a "hybrid controller" that can compensate for large unexpected disturbances.

CHAPTER I

INTRODUCTION

The rapidly increasing use of the digital computer as a means of controlling industrial processes has made possible the use of advanced and optimal control strategies.

Implicit in the implementation of any advanced or optimal control strategy is the development of a dynamic mathematical model of the process or system to be controlled. Most chemical processes are nonlinear, distributed parameter, nondeterministic systems that are very difficult to model. For this reason, empirical, linear models are often developed based on frequency or time domain analysis of input-output data.

This type model is often justified because of the complexity of the system and the fact that advanced control strategy can be developed more easily for these simple models.

If the process is well understood, theoretically derived nonlinear models that are validated by actual process data should be a much more powerful tool. Such theoretical models ususally require less plant data. Extrapolation out of the data range is less risky.

Typical systems where sophisticated models of this type may be justified are distillation columns and chemical reactors. In the case of the distillation column, the form of the model differential

equations may be established by writing material, enthalpy and equilibrium relationships around each stage of the column. These basic equations may then be "tuned-up" by actual column data. For the chemical reactor, unsteady state material and enthalpy balances along with the appropriate kinetic expressions establish the structure of the equations which are then adjusted with plant data.

After the model is developed and validated, optimal control strategy may be formulated. This research will be concerned with this formulation. It will be assumed that the system identification, or the model development, has been accomplished.

Unfortunately, development of optimal control strategies for nonlinear systems is not as straightforward as for simple linear systems. Methods based on the maximum principle usually lead to nonlinear two point boundary value problems which are troublesome to handle numerically. The dynamic programming approach frequently requires excess computer memory.

The purpose of this research is to develop approximate and short-cut methods for the optimal control of nonlinear systems. Since there are so many ways that nonlinearities can occur in system models, a general nonlinear system cannot be studied. For this reason, a variety of "typical" nonlinear systems will be considered. Chemical reactor examples will be chosen throughout this dissertation because they represent one of the most common nonlinear systems that the chemical engineer is faced with.

In Chapter II, the problem of selecting the optimal temperature

or temperature profile for homogeneous, reversible, exothermic reactions is considered. A series of graphs are developed that allow the user to pick off the optimal temperature and conversion attainable for the isothermal operation of batch or plug flow reactors. A graphical technique is also developed for the calculation of optimal temperature profiles. Both of these techniques are suited for a fast "hand" calculation and provide a means to avoid the complicated numerical procedures usually involved in such studies. Most of this work has been published in two recent articles by the author and Groves[1,2].

In Chapter III, a direct finite difference method is developed for the approximate solution of optimal control problems. This reduces the solution of the optimal control problem to the solution of a set of algebraic equations. This method is applied to a wide variety of systems and types of problems. The results are,in all cases, compared to the optimal values. It is shown that a good approximation to the optimal control can be obtained by this method. Much of this work has been accepted for publication as a paper by the author and Groves[3].

The problem of obtaining an approximate optimal closed loop or feedback control algorithm for nonlinear systems is considered in Chapters IV and V. Optimal control theory usually cannot yield a feedback control for nonlinear systems; hence, approximate methods must be considered.

In Chapter IV, a parameter search is used to determine the closed loop control algorithm. This approach is compared to linearization

of the nonlinear system and the application of optimal control theory. This study has been published by the author and Groves[4].

In Chapter V, a more theoretical approach, based on the maximum principle, is used. A "hybrid controller" is developed which can compensate for large and unexpected disturbances.

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CHAPTER II

TEMPERATURE OPTIMIZATION OF CHEMICAL REACTORS

Introduction

The heart of most chemical processes is the reaction step. The difference between profit and loss usually depends most heavily on this step. For this reason much effort should be devoted to the optimal design and operation of the reactor area.

In general, this involves the design of the reaction area such that capital and operating costs are minimized. Obtaining this minimum total cost configuration involves considering such items as materials of construction, instrumentation, catalyst system, operating labor costs, product purification costs and heat or cooling costs. Obviously due to the many variables involved, each reactor system must be considered as a separate case study.

We can however narrow the optimization problem somewhat, thus allowing generalization of results for a whole class of reactions. To do this, we will limit ourselves to selecting the optimal temperature or temperature schedule for homogeneous, exothermic reversible reactions. We shall define optimal as that temperature that maximizes the conversion in a specified reaction time. Aris[1] shows that this is equivalent to minimizing the reaction time necessary to achieve a desired conversion.

Most of the material in this chapter is published in two recent articles by the author and Groves.[2,3]

A brief review of the characteristic differences between endothermic

and exothermic reversible reactions is helpful in appreciating the reasons for considering the reversible exothermic mechanisms.

For most endothermic reversible reactions, an increase in temperature will increase both the reaction rate and the equilibrium conversion. For these reactions, as for most single irreversible reactions, the optimal temperature is the maximum temperature attainable and is set by physical factors such as the temperature the reactor can withstand.

This is not the case for exothermic, reversible reactions (and some heterogeneous catalyzed reactions). An increase in temperature for such reactions causes a decrease in equilibrium conversion. Hence, the best choice of reaction temperature provides a compromise between high reaction velocity at high temperature and high equilibrium conversion at low temperature. It becomes obvious that one should choose a high temperature initially when the reaction is far from equilibrium and a lower temperature as the reaction nears the equilibrium conversion. A simplified procedure to calculate such optimal temperature profiles will be developed in this chapter.

In many cases it is not practical or economical to operate a reactor nonisothermally and follow such an optimal temperature profile. For this reason the optimal isothermal temperature will also be considered. A series of plots will be developed that allow one to pick off the best isothermal temperature and the corresponding conversion attainable as a function of kinetic parameters.

Isothermal Operation

Determination of the optimal isothermal or constant temperature

at which to operate a reactor for carrying out an exothermic reversible reaction is a classical paramter optimization problem.

We are to choose a parameter, T, that will mazimize the conversion, x, obtained during a specified reaction time. The conversion, x, is related to the temperature, T, by a differential equation. The form of this differential equation depends upon the particular reaction mechanism considered.

First Order Illustration: To illustrate this typical problem consider the first order reversible reaction:

$$A \underset{k_r}{\overset{k_f}{\rightleftharpoons}} P \qquad \text{....II-1}$$

where A is the reactant, P is the desired product, k_f is the forward reaction rate constant, and k_r is the reverse reaction rate constant.

For a constant volume batch reactor, the rate of disappearance of A may be expressed by:

$$r_A = -\frac{dC_A}{dt} = k_f C_A - k_r C_P \qquad \text{....II-2}$$

where r_A is the rate of disappearance of A, C_A is concentration of A, C_P is concentration of P, and t is time. Note that the units of k are $t^{-1}C^{1\text{-order}}$. For the above reaction the units of k are t^{-1}.

The variation of rate constant k with temperature is expressed by an Arrhenius relationship as:

$$k_t = k_{fo} \exp(-E_f/RT) \qquad \text{....II-3}$$

$$k_r = k_{ro} \exp(-E_r/RT) \qquad \text{....II-4}$$

where k_{fo} is the frequency factor of the forward reaction, k_{ro} is the frequency factor of the reverse reaction, E_f is the activation energy of the forward reaction and E_r is the activation energy of the reverse reaction, and R is the gas constant. Activation energy, E, and frequency factor, k_o, must normally be obtained from experimental data on rate constant, k, as a function of temperature. References 4 and 5 give typical values for E and k_o for various chemical reactions. The dimensionless conversion is defined as

$$x_A = \frac{C_{AO} - C_A}{C_{AO}} \qquad \text{....II-5}$$

where: C_{AO} = initial concentration of A.

Substitution of equations II-3, II-4, and II-5 into equation II-2 yields:

$$\frac{dx_A}{dt} = k_{fo} \exp(-E_f/RT)(1-x_A) - k_{ro} \exp(-E_r/RT)(x_A) \qquad \text{....II-6}$$

Equation II-6 is our differential equation relating conversion and temperature. The optimization problem may now be stated more precisely. We are to find the temperature, T, that will make the conversion, x_{Af}, at a given reaction time, t_f, a maximum.

We could now solve the problem in a number of ways. A convenient procedure is to integrate equation II-6 from t = 0 to t = t_f and x at t_o to x at t_f, x_{Af}. This results in the rather complicated algebraic expression:

$$x_{Af} = \frac{K_1}{K_2} - \left[\frac{K_1 - K_2 x(t_o)}{K_2}\right] \exp(-K_2 t_f) \qquad \text{....II-7}$$

where: $K_1 = k_{fo} \exp(-E_f/RT)$

$K_2 = k_{fo} \exp(-E_f/RT) + k_{ro} \exp(-E_r/RT)$

This algebraic expression may now be handled by classical optimization theory. Setting the partial of x_{Af} with respect to temperature equal to zero results in the following expression for T:

$$\left\{\frac{1}{1+\frac{k_{ro}}{k_{fo}} \exp\left(\frac{E_f-E_r}{RT}\right)}\right\} - \left\{\left[\exp\left(k_{fo}t_f e^{-E_f/RT} + k_{ro}t_f e^{-E_r/RT}\right)\right]\right.$$

$$\left.\left[\frac{k_{fo}t_f E_f}{T^2} \exp\left(-\frac{E_f}{RT}\right) + t_f k_{ro} \exp\left(-\frac{E_r}{RT}\right) \frac{E_r}{T^2}\right]\right\} = 0 \qquad \text{....II-8}$$

Since equation II-8 is so complicated and must be solved numerically, it is simplier to go back a step and consider equation II-7. We may easily maximize x_{Af} numerically in this equation using a one dimensional search technique. Given K_1, K_2, $x(t_o)$ and t_f we may, by a trial and error procedure, search for the value of T that maximizes x_{Af}. If we assume the initial conversion, $x(t_o)$, is zero, we have three remaining parameters. This, however, is too many to plot conveniently on a single graph.

To overcome this problem, we shall define some additional dimensionless parameters. Let the dimensionless time be defined as:

$$\bar{t} = t/t_f \qquad \text{....II-9}$$

Substitution of equation II-9 into equation II-6 results in:

$$\frac{dx_A}{d\bar{t}} = t_f k_{fo} \exp(-E_f/RT)(1-x_A) - k_{ro}t_f \exp(-E_r/RT)(x_A) \qquad \text{....II-10}$$

We may now group terms as suggested by Millman and Katz[6].

$$\frac{dx_A}{d\bar{t}} = \bar{T}_{11}(1-x_A) - B_{11}(\bar{T}_{11})^a x_A \quad \text{....II-11}$$

where:

$$\bar{T}_{11} = t_f k_{fo} \exp(-E_f/RT) \quad \text{....II-12}$$

$$a = E_r/E_f \quad \text{....II-13}$$

$$B_{11} = t_f k_{ro}/(t_f k_{fo})^a \quad \text{....II-14}$$

Integration of equation II-11 from initial conversion x_{AO} to final conversion x_{Af} and from $\bar{t}$ equals 0 to $\bar{t}$ equals 1, yields:

$$x_{Af} = \frac{1}{\bar{T}_{11}+B_{11}(\bar{T}_{11})^a}\left[\bar{T}_{11} - (\bar{T}_{11}-x_{AO}z)e^{-z}\right] \quad \text{....II-15}$$

where:

$$z = \bar{T}_{11} + B_{11}(\bar{T}_{11})^a \quad \text{....II-16}$$

For the initial conversion, x_{AO} equal to zero equation, II-15, is an algebraic expression relating dimensionless temperature, $\bar{T}_{11}$, to the final conversion, x_{Af}. There are now only two parameters, B_{11} and a.

Maximizing equation II-15 was accomplished by using a golden section search technique[7] on the digital computer. The program for this method can be found in Appendix A. The optimal value of $\bar{T}_{11}$ is plotted in Figure II-1 against B_{11} with "a" as a parameter. The

optimal conversion, x_{Af}, obtained by operating at the corresponding optimal temperature, is shown in Figure II-2.

A development similar to that shown above can be applied to other reversible reaction mechanisms. The dimensionless rate expression for some common mechanisms are shown below:

Second Order Forward - Second Order Reverse: $A+B \rightleftarrows P+S$

$$\frac{dx_A}{d\bar{t}} = \bar{T}_{22}(1-x_A)(M-x_A) - B_{22}(\bar{T}_{22})^a x_A^2 \qquad \text{....II-17}$$

where:

$$\bar{T}_{22} = t_f k_{fo} C_{AO} \exp(-E_f/RT) \qquad \text{....II-18}$$

$$B_{22} = (k_{ro} t_f C_{AO})/(k_{fo} t_f C_{AO})^a \qquad \text{....II-19}$$

$$M = C_{BO}/C_{AO}$$

First Order Forward - Second Order Reverse: $A \rightleftarrows P+S$

$$\frac{dx_A}{d\bar{t}} = \bar{T}_{12}(1-x_A) - B_{12}(\bar{T}_{12})^a x_A^2 \qquad \text{....II-20}$$

where:

$$\bar{T}_{12} = k_{fo} t_f \exp(-E_f/RT) \qquad \text{....II-21}$$

$$B_{12} = k_{ro} t_f C_{AO}/(k_{fo} t_f)^a \qquad \text{....II-22}$$

Second Order Forward - First Order Reverse: $A+B \rightleftarrows P$

$$\frac{dx_A}{d\bar{t}} = \bar{T}_{21}(1-x_A)(M-x_A) - B_{21}(\bar{T}_{21})^a x_A \qquad \text{....II-23}$$

where:

$$\bar{T}_{21} = t_f k_{fo} C_{AO} \exp(-E_f/RT) \qquad \text{....II-24}$$

$$B_{21} = k_{ro} t_f / (C_{AO} t_f k_{fo})^a \qquad \text{....II-25}$$

$$M = C_{BO}/C_{AO}$$

Dimensionless parameters defined above are summarized in Table II-1.

Figures II-3 through II-8 are the optimal temperature and corresponding conversion graphs for second order forward and second order reverse reactions. Figures II-9 through II-14 are the corresponding plots for second order forward and first order reverse reactions.

Note that the first subscript on the dimensionless parameters corresponds to the order of the forward reaction and the second subscript corresponds to the order of the reverse reaction. Also note that although the preceding analysis assumed a batch reactor, the equations and figures apply equally well to a plug flow tubular reactor provided the charge in volume accompanying the reaction is small. It is only necessary to interpret the variable t or residence time in the tubular reactor.

Figures II-1 through II-14 are the principle results of this

Table II-1

Dimensionless Parameters for Different Mechanisms

Reaction Order			
Forward	Reverse		
1	1	$B_{11} = \frac{k_{ro} t_f}{(k_{fo} t_f)^a}$	$\overline{T}_{11} = t_f k_{fo} e^{-E_f/RT}$
2	1	$B_{21} = \frac{k_{ro} t_f}{(C_{AO} t_f k_{fo})^a}$	$\overline{T}_{21} = t_f k_{fo} C_{AO} e^{-E_f/RT}$
2	2	$B_{22} = \frac{k_{ro} t_f C_{AO}}{(C_{AO} t_f k_{fo})^a}$	$\overline{T}_{22} = t_f k_{fo} C_{AO} e^{-E_f/RT}$

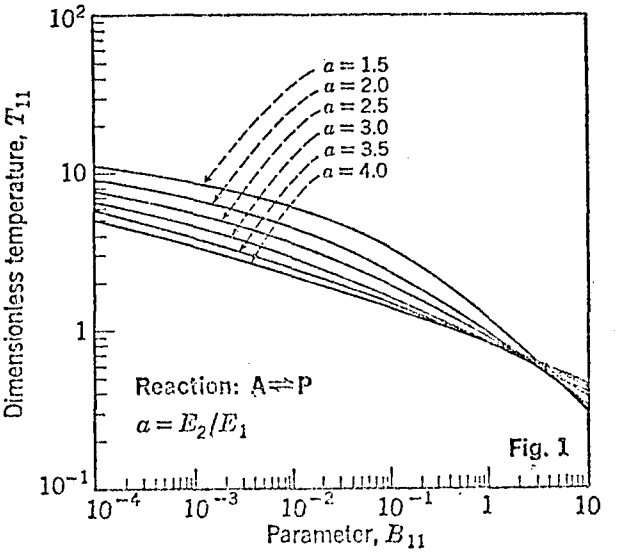

Figure II-1

Dimensionless T_{11} vs B_{11}

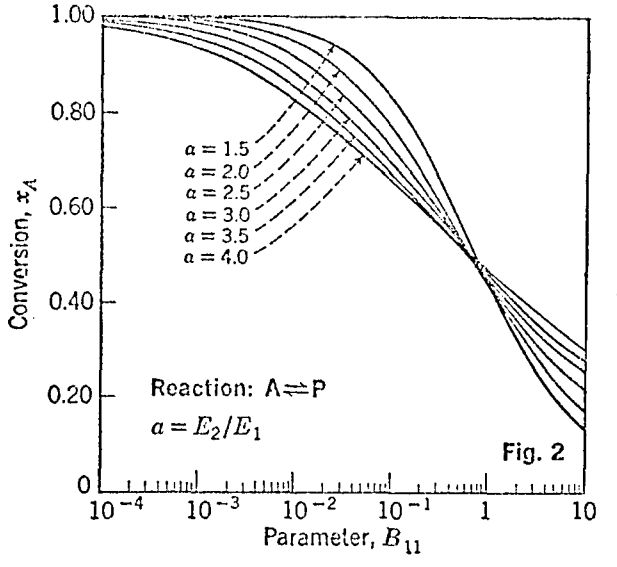

Figure II-2

Conversion vs B_{11}

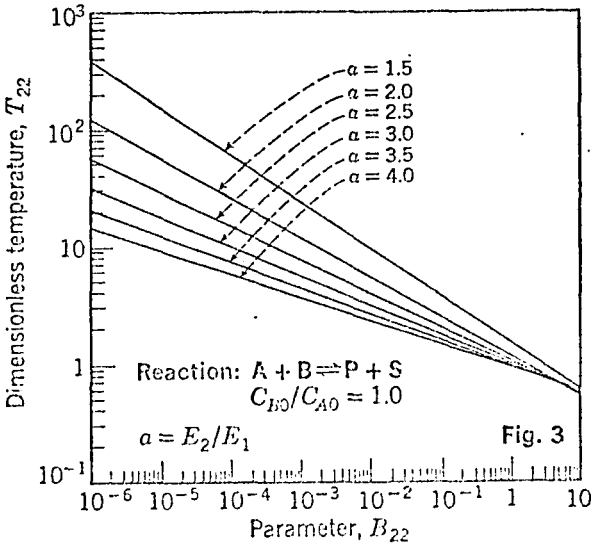

Figure II-3

Dimensionless T_{22} vs B_{22}

$C_{BO}/C_{AO} = 1.0$

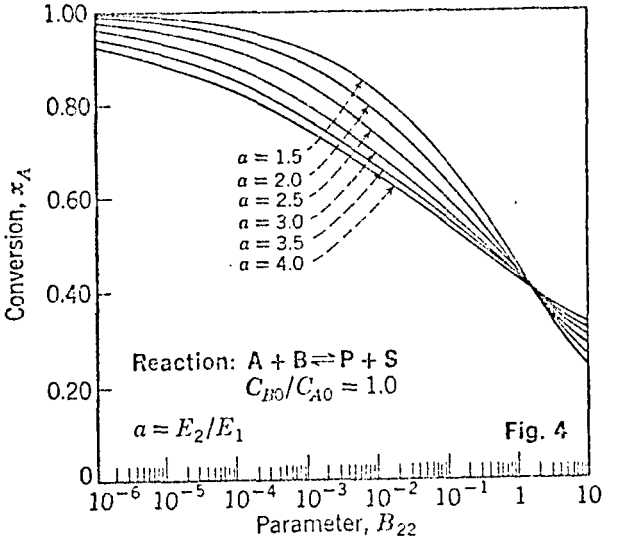

Figure II-4

Conversion vs B_{22}

$C_{BO}/C_{AO} = 1.0$

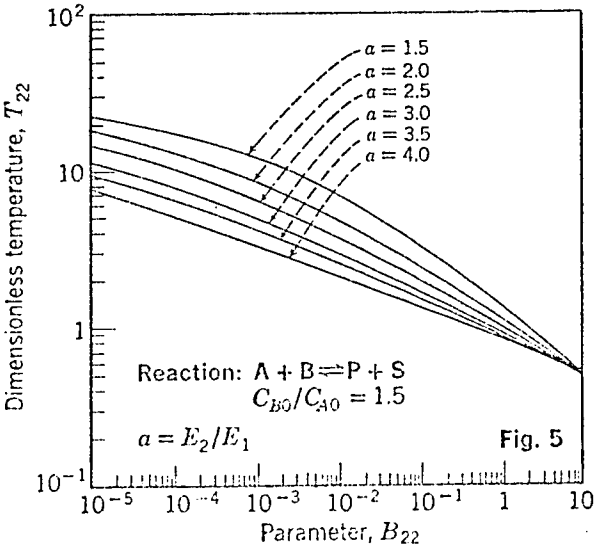

Figure II-5

Dimensionless T_{22} vs B_{22}

$C_{BO}/C_{AO} = 1.5$

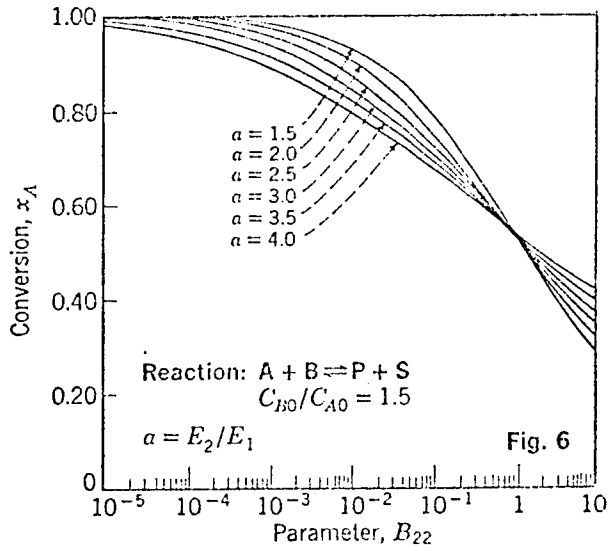

Figure II-6

Conversion vs B_{22}

$C_{BO}/C_{AO} = 1.5$

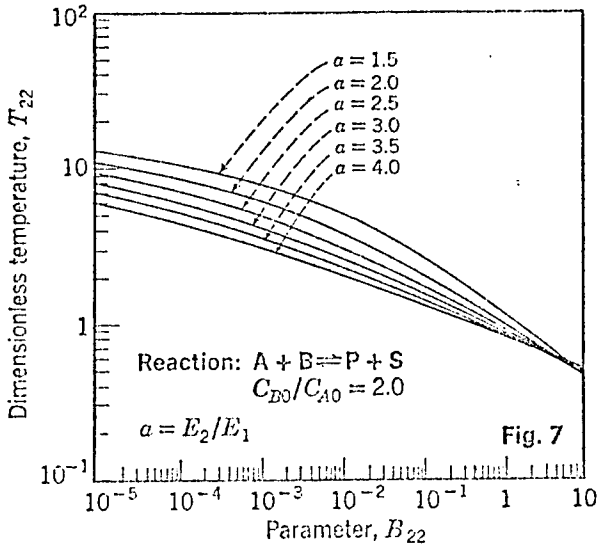

Figure II-7

Dimensionless T_{22} vs B_{22}

$C_{BO}/C_{AO} = 2.0$

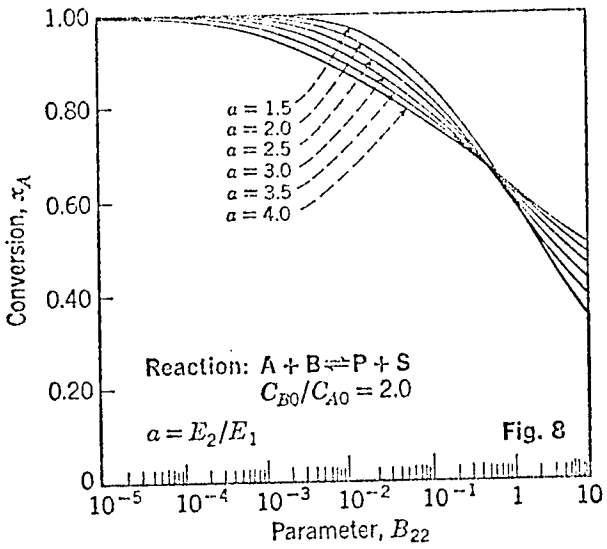

Figure II-8

Conversion vs B_{22}

$C_{BO}/C_{AO} = 2.0$

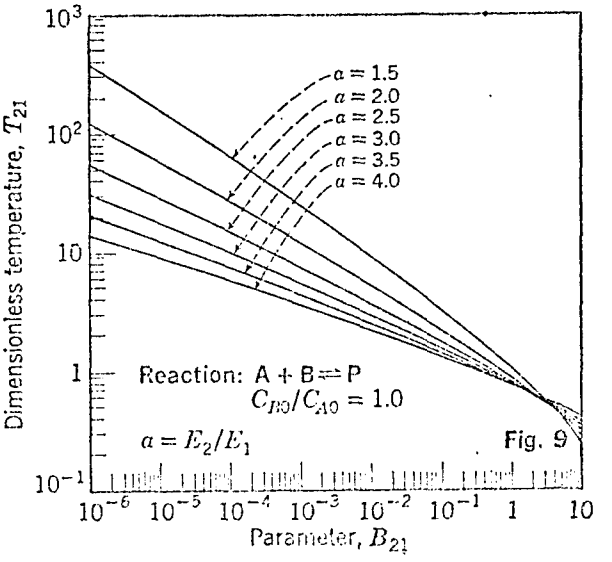

Figure II-9

Dimensionless T_{21} vs B_{21}

$C_{BO}/C_{AO} = 1.0$

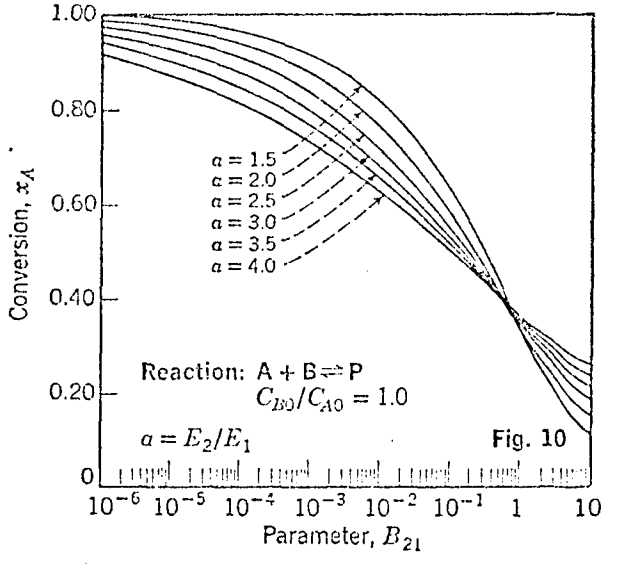

Figure II-10

Conversion vs B_{21}

$C_{BO}/C_{AO} = 1.0$

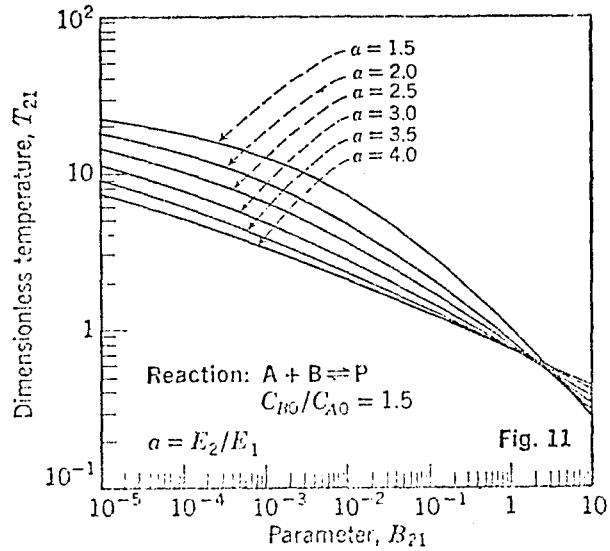

Figure II-11

Dimensionless T_{21} vs B_{21}

$C_{BO}/C_{AO} = 1.5$

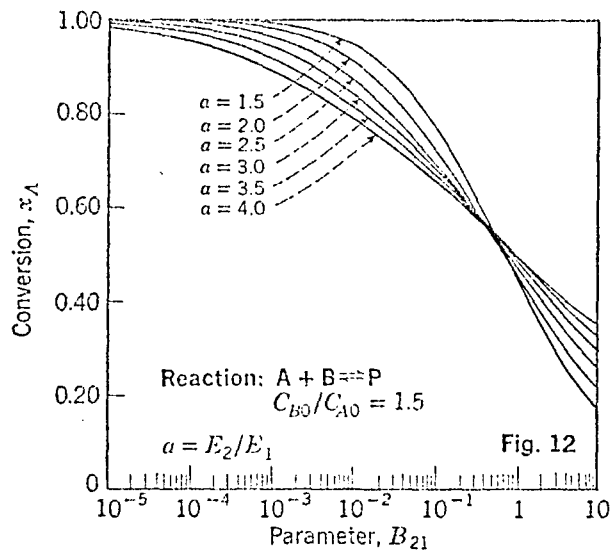

Figure II-12

Conversion vs B_{21}

$C_{BO}/C_{AO} = 1.5$

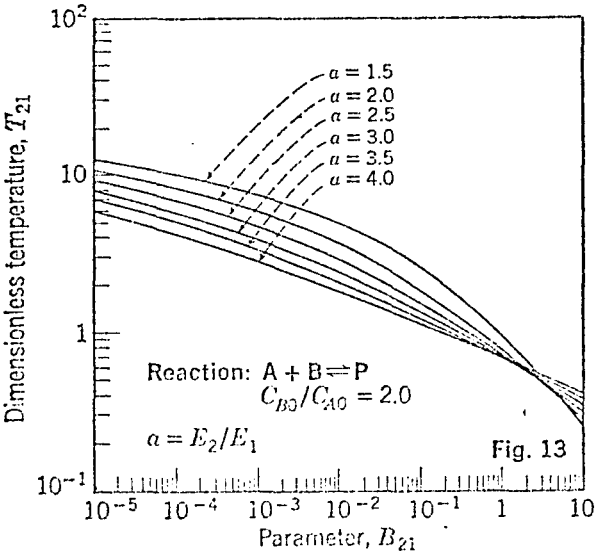

Figure II-13

Dimensionless T_{21} vs B_{21}

$C_{BO}/C_{AO} = 2.0$

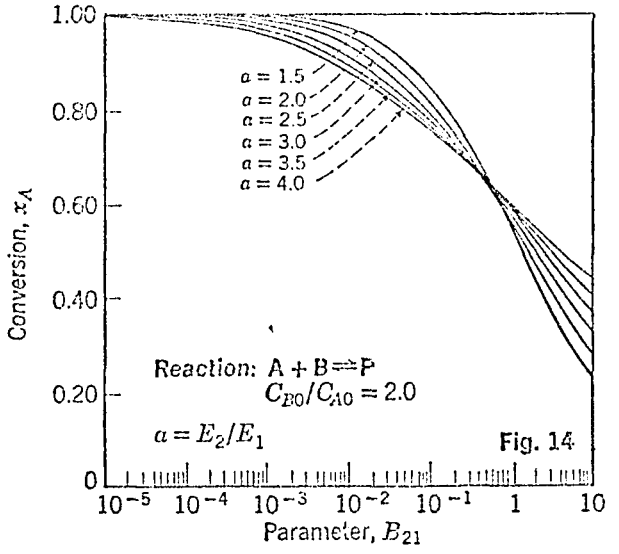

Figure II-14

Conversion vs B_{21}

$C_{BO}/C_{AO} = 2.0$

study. These generalized graphs may be used to rapidly determine the optimal temperature and corresponding conversion attainable. The utilization of these graphs will now be illustrated.

Use of Graphs: There are two approaches to solving for the optimal isothermal temperature using these graphs. These are:

1. Specify desired conversion and use the conversion vs. B plot to obtain B. From B and kinetic parameters calculate reaction time t_f using definition of B in Table II-1. From dimensionless temperature vs. B plot obtain $\bar{T}$ and calculate actual temperature, from definition in Table II-1.
2. Specify reaction time. Calculate B using definition in Table II-1 and obtain $\bar{T}$ from $\bar{T}$ vs. B. Convert to actual temperature using the definition of $\bar{T}$ from Table II-1. From plot of conversion of A vs. B obtain the optimal conversion.

A simple example will illustrate the second approach:

A given reaction may be approximated by the first order reversible reaction $A \rightleftarrows B$. The reaction is carried out in a tubular plug flow reactor. Flow velocity through the reactor is 5 ft/sec and tube length is 50 ft. Thus, the reaction time is 10 sec.

Kinetic parameters are:

$k_{10} = 2.5 \times 10^5$/hr

$k_{20} = 2.0 \times 10^7$/hr

$E_f = 10{,}000$ BTU/lb mole

$E_r = 20{,}000$ BTU/lb mole

Find the optimal isothermal temperature for this reactor and the conversion attainable.

1. Calculate dimensionless parameters:

$$a = E_r/E_f = 20{,}000/10{,}000 = 2.0$$

$$B_{II} = k_{ro}t_f/(k_{fo}t_f)^a = \frac{(2\times10^7)(10/3600)}{[(2.5\times10^5)(10/3600)]^2} = 0.115$$

2. From Figure II-1 obtain:

$$\bar{T}_{II} = 2.3$$

3. Calculate T:

$$T = \frac{-E_f}{R\ln\frac{\bar{T}_{11}}{t_f k_{fo}}} = \frac{-10{,}000}{1.987\ \ln\frac{(2.3)}{(2.78\times10^{-3})(2.5\times10^5)}} = 884^{\circ}R$$

4. From Figure II-2 obtain:

$$x_A = 0.75$$

Variable Temperature Operation

As has been mentioned, the optimal way to carry out a reversible exothermic reaction is to operate at a high temperature initially and reduce the temperature as equilibrium is approached. Calculation of such an optimal temperature profile is a typical variational or functional optimization problem. That is, we desire an optimal function, T(t), and not just an optimal value of a parameter as was the case in the previous isothermal study.

Problems such as this have been solved by different variational methods such as the calculus of variations[7], dynamic programming[1] and

the maximum principle of Pontryagin[8]. To illustrate the use of the maximum principle, which will be referred to extensively in this dissertation, the optimal temperature profile will be determined for a simple reversible reaction. The example will be similar to that considered by Fan[8].

After illustration of the maximum principle route to solution, a simplified graphical technique will be developed. This technique is suited for a fast "hand" calculation and can be used for any reversible mechanism.

Application of the Maximum Principle: Let us reconsider the first order reversible reaction:

$$A \underset{k_r}{\overset{k_f}{\rightleftarrows}} P \qquad \text{....II-26}$$

For the reaction carried out in a batch reactor the system dynamics may be described by equation II-6. In the variable temperature case, however, temperature is an unknown function of time. Therefore, equation II-6 may be written as:

$$\frac{dx_A}{dt} = k_{fo} \exp(-E_f/RT(t))(1-x_A) - k_{ro} \exp(-E_r/RT(t)) (x_A) \text{....II-27}$$

where: $T(t)$ = the desired optimal temperature function.

At this point, we must specify what is considered an optimal control or temperature function. For this example, the reaction time will be set

and the conversion achieved at that time is to be maximized.

To restate the problem more precisely, we wish to find the temperature function T(t) that will "drive" the system described by equation II-27 such that the final conversion is maximized.

The following application of the maximum principle will be presented only as an illustration. Proofs and details of this formulation can be found in Athans[9], Fan[8] and Koppel[10].

According to the maximum principle, the optimal control is one that minimizes the Hamiltonian which is an adjoined cost function. For our problem, the Hamiltonian may be written as:

$$H = -x(t_f) + \lambda(t)[k_{fo}(1-x)\exp(-E_f/RT) - k_{ro}x\exp(-E_r/RT)] \quad \text{....II-28}$$

where $\lambda(t)$ is a Lagrange multiplier or costate variable. The necessary conditions for H to be extremal are:

$$\frac{d\lambda(t)}{dt} = -\frac{\partial H}{\partial x} = 1 + \lambda[k_{fo}\exp(-E_f/RT(t)) + k_{ro}\exp(-E_r/RT)] \quad \text{....II-29}$$

$$\lambda(t_f) = 1$$

$$\frac{dx}{dt} = \frac{\partial H}{\partial \lambda} = k_{fo}\exp(-E_f/RT(t))(1-x) - k_{ro}\exp(-E_r/RT(t))\,x \quad \text{....II-30}$$

$$x(t_o) = 0 \text{ (specified)}$$

$$\frac{\partial H}{\partial T} = 0 = \frac{\lambda_1}{RT(t)^2}[k_{fo}(1-x)E_f\exp(-E_f/RT^*) + E_r x\exp(-E_r/RT^*)] \quad \text{....II-31}$$

The differential equations II-29 and II-30 are typical of those encountered in application of the maximum principle. They represent a two point boundary value problem in that the intial condition on one equation is specified along with the final condition on the other. Such equations, in general, require difficult trial and error solutions. Much of the remainder of this dissertation will be concerned with such problems. Approximate solutions to such equations will be considered as will fast hybrid computer techniques for their solution.

In this simple example, however, we can avoid solution of the two point boundary value problem. This is because the adjoint or costate variable, λ, drops out of the solution.

Solving equation II-31 for the optimal temperature function, $T^*(t)$, results in:

$$T^*(t) = \frac{E_r - E_f}{R \ln\left[\left(\frac{k_{ro}E_r}{k_{fo}E_f}\right)\left(\frac{x}{1-x}\right)\right]} \qquad \text{....II-32}$$

which is only a function of the state variable, x. Substitution of equation II-32 into equation II-30 yields:

$$\frac{dx}{dt} = k_{fo}(1-x)\left[\left(\frac{k_{ro}E_r}{k_{fo}E_f}\right)\left(\frac{x}{1-x}\right)\right]^{-\left(\frac{E_f}{E_r-E_f}\right)} - k_{ro}x\left[\left(\frac{k_{ro}E_r}{k_{fo}E_f}\right)\left(\frac{x}{1-x}\right)\right]^{-\left(\frac{E_r}{E_r-E_f}\right)}$$

....II-33

Equation II-33 was integrated numerically from t equal zero to t equal thirty using the same parameters that were used in the isothermal example. This results in the optimal conversion versus time relationship shown in Figure II-15. The optimal temperature relationship of Figure II-16

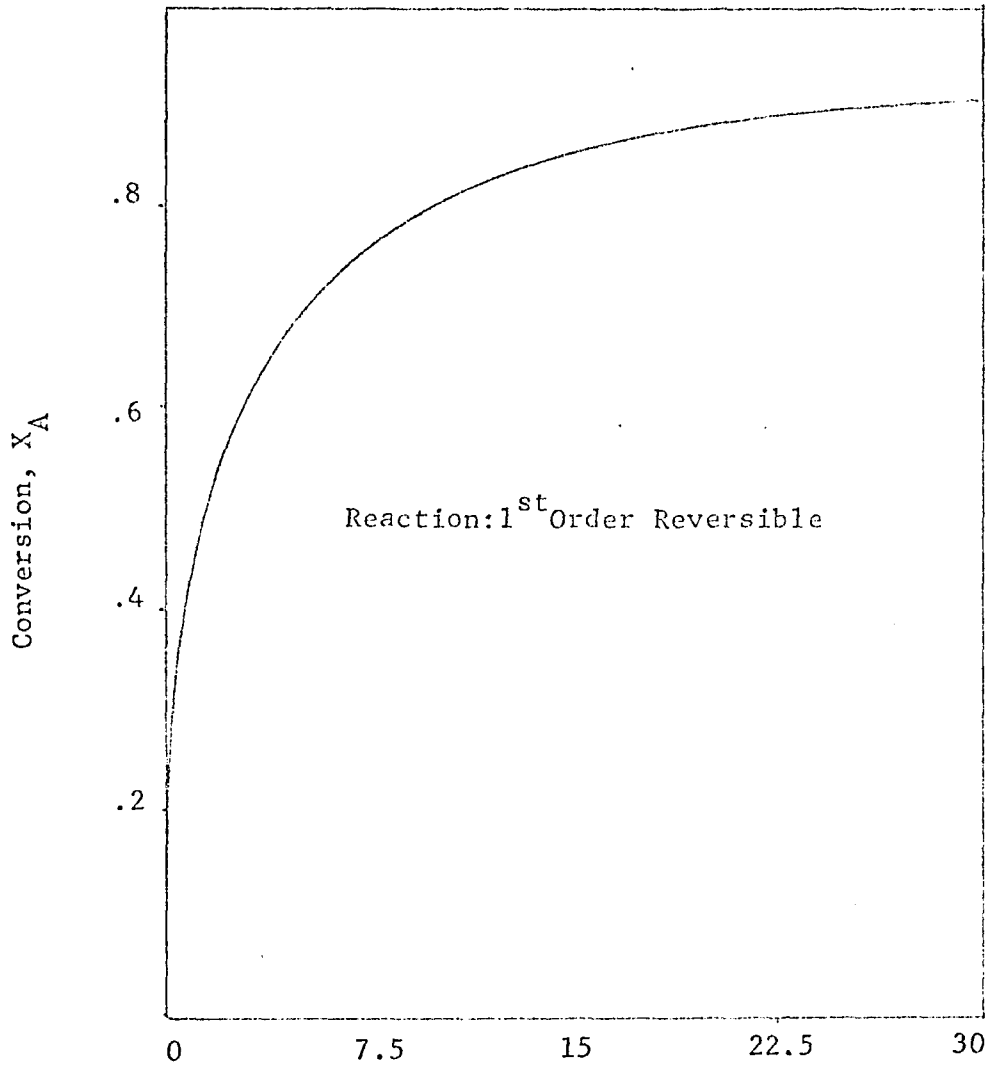

Figure II-15
Optimal Conversion vs Time

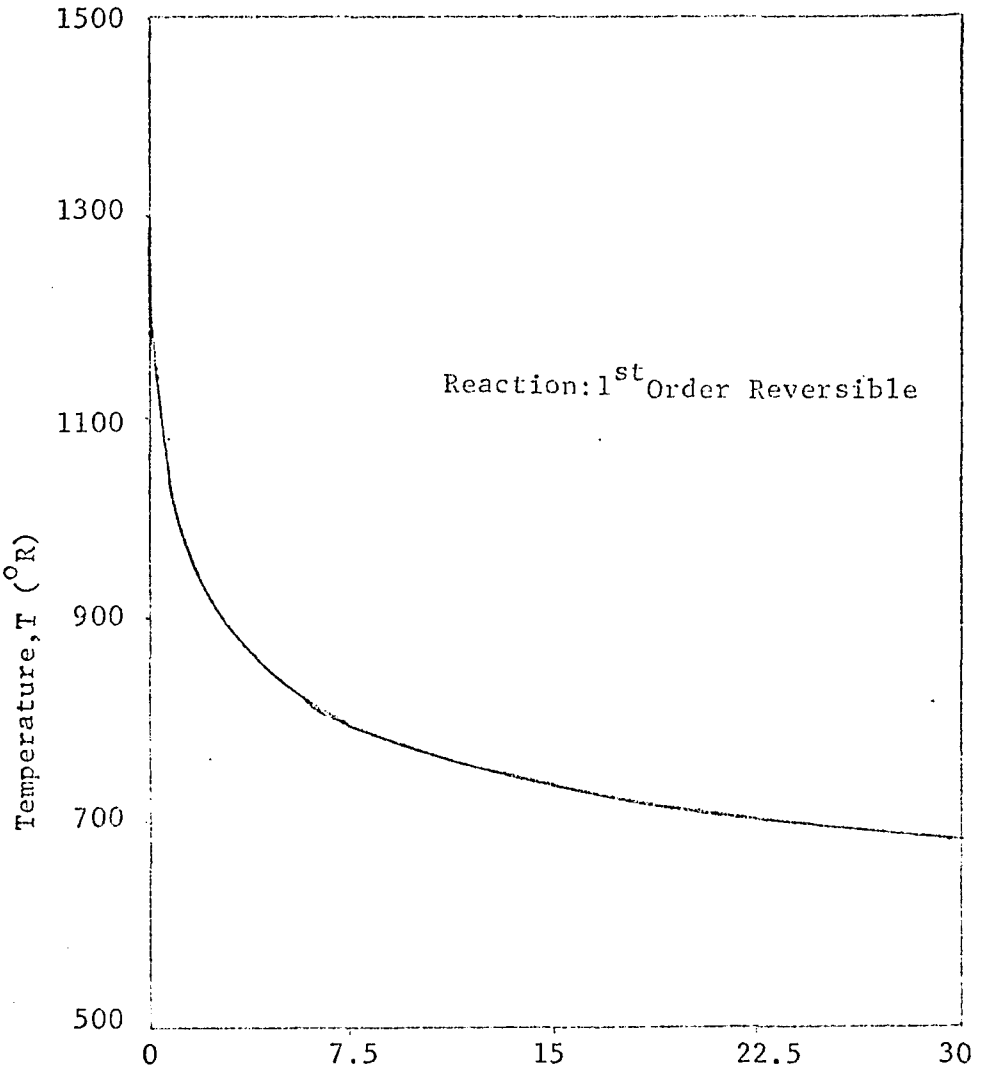

Figure II-16
Optimal Temperature vs Time

is obtained by simultaneous solution of equations II-33 and II-32.

Temperature Constraints: Notice that at very small values of time the temperature approaches an infinite value. Obviously there is a maximum temperature beyond which we cannot operate. This is set by physical and economic factors such as materials of construction, stability of reacting materials, cost of heating and safety considerations. The temperature constraint is handled by operating at the maximum temperature possible until a conversion is reached that corresponds to the maximum temperature point on the theoretical temperature conversion diagram. Figure II-17 is a typical optimal temperature versus conversion diagram and illustrates this point. The A-B-C segment of the curve is the constrained path. Figure II-18 shows the corresponding optimal temperature versus time. If a minimum temperature constraint is placed on the system it is handled in the same way.

Development of a Simplified Graphical Procedure: The solution via maximum principle illustrated above is rather complex even for this simple first order mechanism. It becomes even more complex for other mechanisms. For this reason, a simplified graphical procedure will be developed that is suited for a fast "hand" calculation of the optimal temperature profile for any reversible reaction mechanism.

The development will be illustrated by a simple first order reaction such as equation II-1. Using dimensionless conversion defined in equation II-5 and the Arrhenius temperature relationship of equations II-3 and II-4, we may write the reaction rates as:

$$r_A = C_{AO}\frac{dx_A}{dt} = k_{fo}\exp(-E_f/RT)C_{AO}(1-x_A) - k_{ro}\exp(-E_r/RT)C_{AO}x_A \quad \text{....II-34}$$

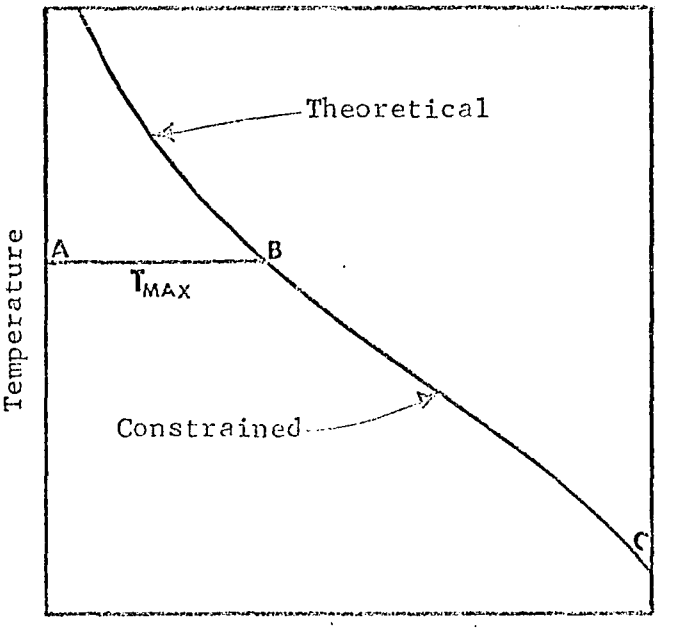

Figure II-17

Typical Optimal Temperature
vs Conversion

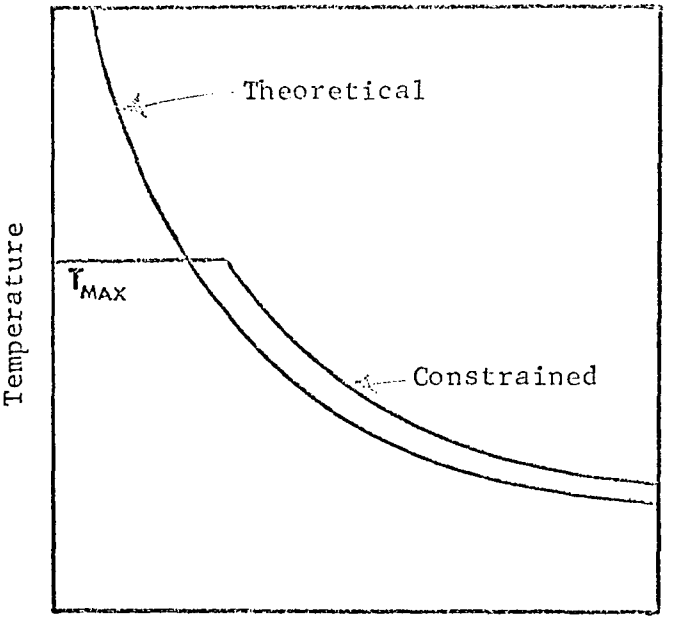

Figure II-18
Effect of Constraint on
Temperature Profile

Aris[1] demonstrates that for single reactions maximization of rate at every point along the reaction path is sufficient to maximize conversion. Hence, to maximize rate as a function of temperature we may write:

$$\frac{\partial r}{\partial T} = a_1 k_{fo} E_f \exp(-E_f/RT) - a_2 k_{ro} E_r \exp(-E_r/RT) = 0 \quad \ldots.II\text{-}35$$

where: $a_1 = C_{AO}(1-x_A)$

$a_2 = C_{AO} x_A$

solving equation II-35 for optimal temperature, T^*, yields:

$$\exp\left(\frac{-B_1}{T^*}\right) = B_2 B_3 \quad \ldots.II\text{-}36$$

where:

$$B_1 = \frac{E_f - E_r}{R} \quad \ldots.II\text{-}37$$

$$B_2 = \frac{E_r k_{ro}}{E_f k_{fo}} \quad \ldots.II\text{-}38$$

$$B_3 = \frac{a_2}{a_1} \quad \ldots.II\text{-}39$$

$$B_2 B_3 > 1$$

Note that B_1 and B_2 are constants and are valid for all reversible mechanisms. B_3 is a function of conversion and depends upon the particular mechanism. Table II-2 contains the parameter B_3 for different reaction mechanisms. For less common reversible mechanism, B_3 may be

Table II-2

Parameter B_3 for Different Mechanisms

Mechanism	B_3
$A \rightleftarrows P$	$\frac{x_A}{1-x_A}$
$A+B \rightleftarrows P+S$	$\frac{x_A^2}{(1-x_A)(M-x_A)}$ *
$A \rightleftarrows P+S$	$\frac{C_{AO}x_A^2}{(1-x_A)}$
$A+B \rightleftarrows P$	$\frac{x_A}{C_{AO}(1-x_A)(M-x_A)}$

* $M = C_{BO}/C_{AO}$

derived as was done above.

Equation II-36 is plotted in Figure II-19 as inverse temperature versus B_2B_3 with B_1 as a parameter. This provides an easy way to obtain the optimal temperature at given conversions for any reversible exothermic reaction. The temperature-time relationship is obtained by numerical or graphical integration of equation II-34 or its equivalent. This procedure will be illustrated by an example.

Example: Consider the following first order reversible reaction:

$$A \rightleftarrows P$$

The kinetic parameters are:

$k_{fo} = 69.5/\text{min}$

$k_{ro} = 5555/\text{min}$

$E_f = 10{,}000$ BTU/lb moles

$E_r = 20{,}000$ BTU/lb moles

The reaction is carried out in a batch reactor. The materials of construction are such that the maximum temperature the reactor can safely withstand is $1500^{\circ}R$. A conversion of reactant A of 0.8 is desired. Find the optimal temperature as a function of conversion and time. The procedure is as follows:

1. Calculate parameters B_1 and B_2:

$$B_1 = (E_f - E_r)/R = 10{,}000/1.987 = -5033^{\circ}R$$

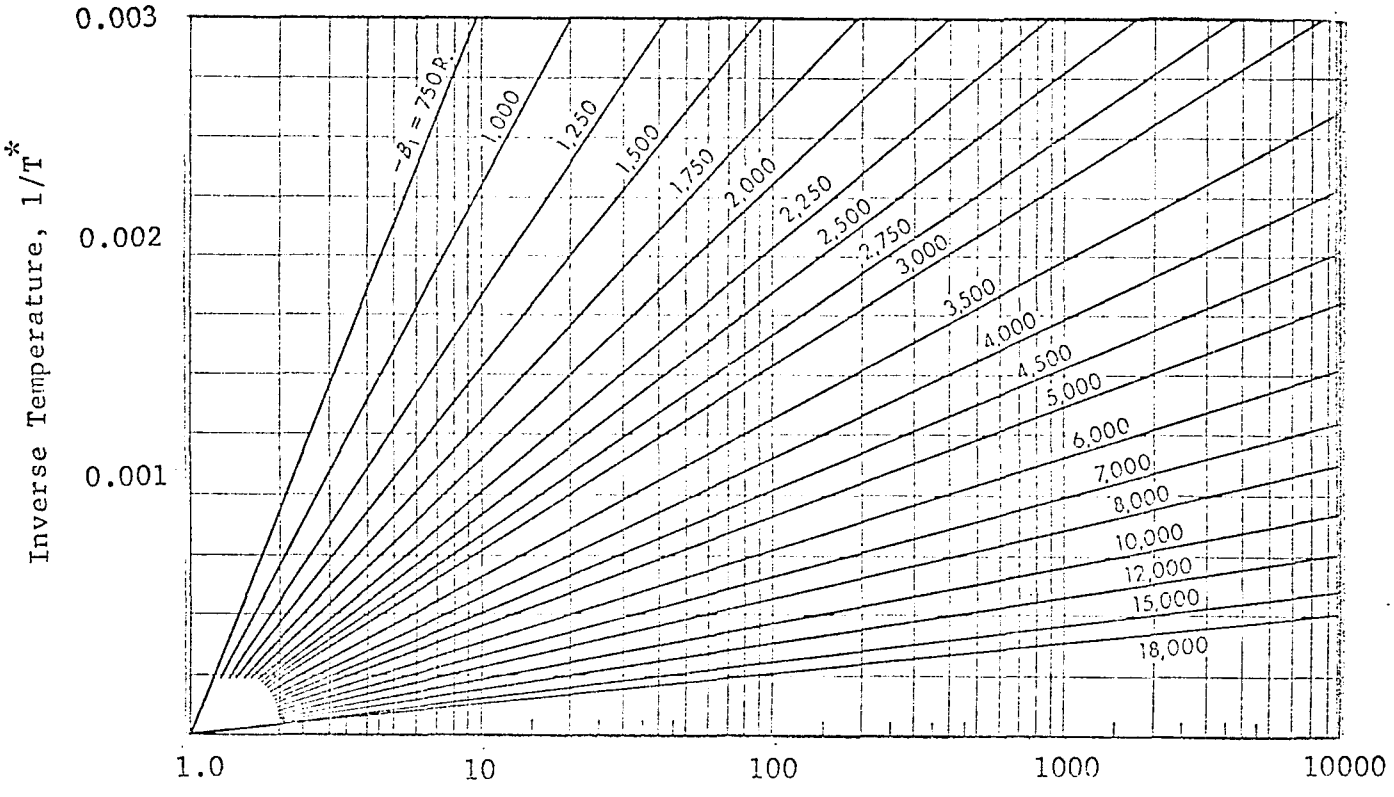

Figure II-19

Inverse Optimal Temperature
vs B_2B_3

$$B_2 = \frac{E_r k_{ro}}{E_f k_{fo}} = \frac{20{,}000 \times 5555}{10{,}000 \times 69.5} = 160$$

2. Obtain expression for B_3 from Table II-2. Look up B_2B_3 in Figure II-19 corresponding to the maximum temperature. Calculate conversion at this point:

$B_2B_3 = 28.5$ @ $T = 1500^{\circ}R$ (From Figure II-19)

$B_3 = 28.5/160 = .178$

$x = B_3/(1+B_3) = .178/1.178 = .152$

3. Use Figure II-19 with B_1, B_2, and B_3 to look up optimal temperature versus conversion for conversion between .152 and 0.8. The results are:

x_A	$B_3 = \frac{x_A}{1-x_A}$	B_2B_3	$T^*(^{\circ}R)$
.151	.178	28.5	1500
.2	.250	40	1370
.4	.670	107	1080
.6	1.5	246	920
.8	4.0	640	780

4. The approximate temperature-time relationship is obtained by graphical integration of equation II-34 using the corresponding temperatures and conversions from Step 3. Figure II-20 illustrates this procedure. The resulting

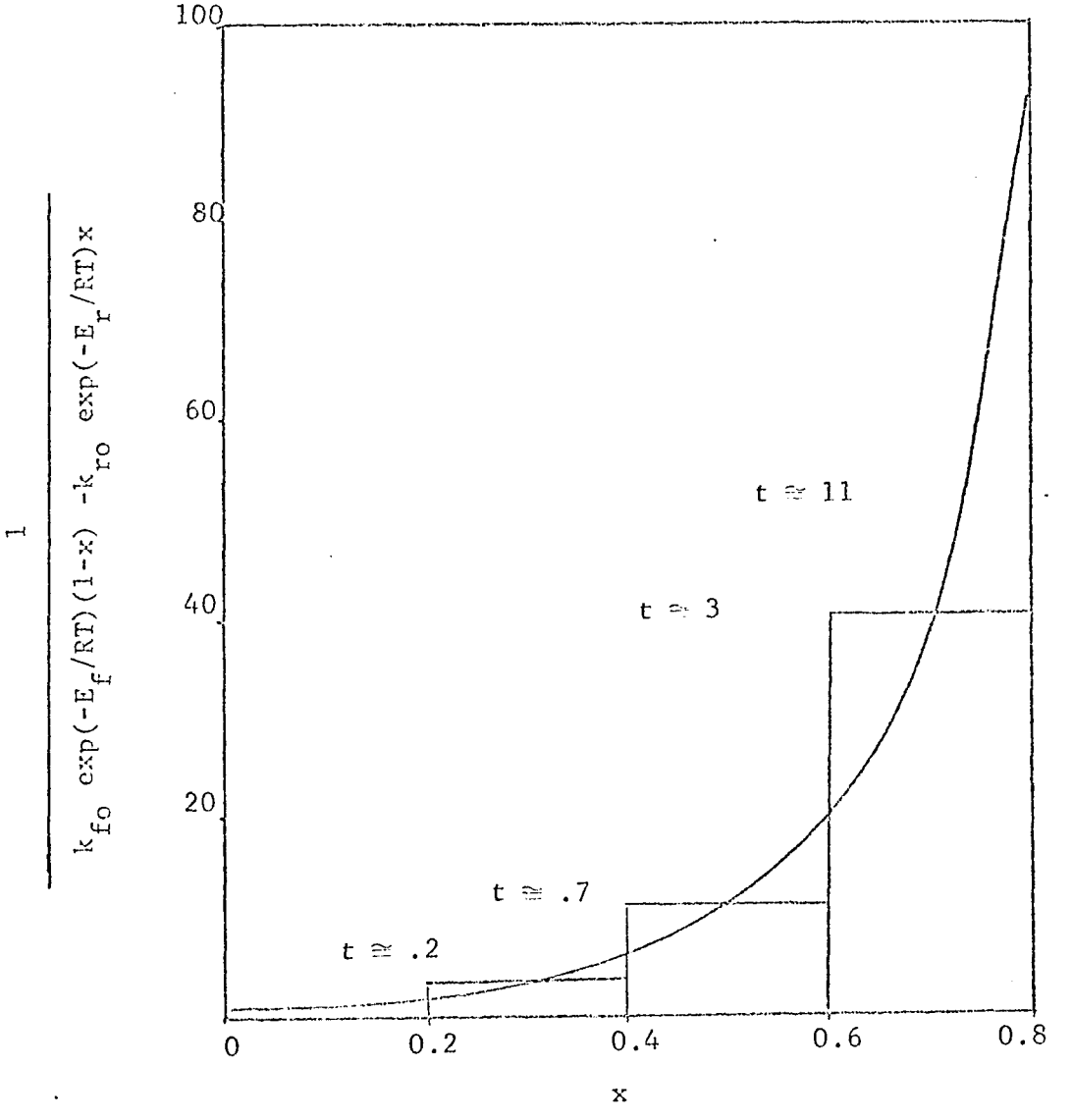

Figure II-20
Graphical Intergration of Equ (34)

optimal conversion-temperature-time relationship is:

x_A	$T^*(^oR)$	Time (min)
0	1500	0
.152	1500	0.1
.2	1370	0.2
.4	1080	0.7
.6	920	3.0
.8	780	11.0

The use of the graphs has been illustrated by a batch reactor. The same method may be used for a tubular plug flow reactor provided that volume changes associated with the reaction are negligible. It is only necessary to interpret time in the above discussion as residence time in the tubular reactor.

Conclusion

The graphs developed in this chapter provide the engineer with a tool for rapid determination of the best temperature or temperature profile for homogeneous, exothermic, reversible reations. They are designed for a fast "hand" calculation and provide a means to avoid the complicated numerical procedures usually involved in such studies.

The development illustrates two classic optimization problems involving nonlinear systems. The first is a parameter optimization where we search for a single parameter, temperature, that will maximize the

yield. The second is a variational problem where we desire an optimal function, $T^*(t)$, that maximizes yield. The variational problem is typical of optimal control problems.

In the following chapter an alternate procedure for handling variational or optimal control problems will be considered. The method, termed a "direct finite difference" method, will be developed and applied to a variety of linear and nonlinear optimal control problems.

Nomenclature

B_1--------Parameter defined by Equation II-37

B_2--------Parameter defined by Equation II-38

B_3--------Parameter defined by Equation II-39

$B_{n,m}$------Parameter defined in Table II-1

C_A--------Concentration of reactant A

C_P--------Concentration of product P

C_{AO}-------Initial concentration of A

E_f--------Activation energy of forward reaction

E_r--------Activation energy of reverse reaction

H---------Hamiltonian function

K_1--------Parameter defined by Equation II-7

K_2--------Parameter defined by Equation II-7

M---------Initial concentration ratio

R---------Gas constant

T---------Absolute temperature

$T^*(t)$-----Optimal temperature function

$T_{n,m}$------Dimensionless temperature defined in Table II-1

a---------Parameter defined by Equation II-13

k_f--------Forward reaction rate constant

k_r--------Reverse reaction rate constant

k_{fo}-------Frequency factor of forward reaction

k_{ro}-------Frequency factor of reverse reaction

t---------Time

t_o--------Initial time

t_f--------Final reaction time

$\bar{t}$---------Dimensionless time defined by Equation II-9

x_A--------Dimensionless conversion of A defined by Equation II-5

z---------Parameter defined by equation II-16

λ---------Adjoint or costate variable

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CHAPTER III

A DIRECT FINITE DIFFERENCE METHOD FOR OPTIMAL CONTROL PROBLEMS

Introduction

The theory necessary to solve optimal control problems has been known for many years. Use of this theory to solve practical problems has lagged behind. This is partly due to the computational difficulties involved in getting a numerical solution. On the one hand, methods based on the maximum principle lead usually to two point boundary value problems, which are troublesome to handle numerically. On the other hand, the dynamic programming method frequently requires excessive computer memory.

Because of these difficulties an approximate numerical method that is easy to implement is very desirable. This chapter describes such a method. We refer to it as a direct method because it deals directly with the function to be minimized. This approach has been known for many years and is based on the Rayleigh-Ritz method for problems in the calculus of variations[1]. It has recently been applied to variational problems by Greenspan[2]. An adaptation for use on optimal control problems has been suggested by Sage[3]. The purpose of this chapter is to apply the direct finite difference approach to a variety of typical optimal control problems.

Illustration of the Direct Method

The method is called direct because it deals directly with the function to be minimized. To illustrate this problem consider a typical problem in the calculus of variations:

The problem is to find a function y(t) that minimizes (or maximizes) the following integral:

$$J = \int_a^b F(t,y,\dot{y})dt \qquad \ldots.III\text{-}1$$

where: $\dot{y} = \frac{dy(t)}{dt}$

subject to the boundary conditions:

$$y = A \quad \text{at} \quad t = a \qquad \ldots.III\text{-}2$$

$$y = B \quad \text{at} \quad t = b \qquad \ldots.III\text{-}3$$

The calculus of variations approach to this problem yields the Euler equation:

$$\frac{\partial F}{\partial y} - \frac{d}{dt}\frac{\partial F}{\partial \dot{y}} = 0 \qquad \ldots.III\text{-}4$$

Application of the Euler equation to our problem generally results in a nonlinear, second order, ordinary differential equation that must be solved numerically to obtain the optimum function, $y^*(t)$. The calculus of variations is considered an indirect solution method because we solve the Euler equation for the optimal function and not the original problem defined by equation III-1.

A direct method would "directly" solve the original problem defined by equation III-1. Greenspan points out that numerically it is

often easier to solve the fundamental problem defined by equation III-1 than that resulting from equation III-4.

One of the oldest direct methods was developed independently by Ritz and Rayleigh. For a detailed discussion of this method, see references 1 and 3. The direct finite difference method is an adaptation of the Rayleigh-Ritz method.

Again, consider the typical problem in the calculus of variations defined by equation III-1 for an illustration of the finite difference method. If we divide the interval a to b into N equal parts and define $\Delta t = \frac{b-a}{N}$, we may approximate the functional J numerically. Rectangular integration is used with forward difference approximation of the derivatives as follows:

$$
\begin{aligned}
J \approx & \left\{F\left(t_o, y^o, \frac{y^1 - y^o}{\Delta t}\right)\right\} \Delta t \\
& + \left\{F\left(t_1, y^1, \frac{y^2 - y^1}{\Delta t}\right)\right\} \Delta t \\
& + \left\{F\left(t_2, y^2, \frac{y^3 - y^2}{\Delta t}\right)\right\} \Delta t \\
& \vdots \\
& + \left\{F\left(t_{N-1}, y^{N-1}, \frac{y^N - y^{N-1}}{\Delta t}\right\}\right. \Delta t
\end{aligned}
\qquad \ldots\ldots \text{III-5}
$$

Or simply:

$$
J \approx \Delta t \sum_{i=1}^{n} F\left(t_{i-1}, y^{i-1}, \frac{y^i - y^{i-1}}{\Delta t}\right) \qquad \ldots\ldots \text{III-6}
$$

Note that from the boundary conditions are:

$$y^{o} = A \qquad \ldots.III\text{-}7$$

$$y^{N} = B \qquad \ldots.III\text{-}8$$

Hence, there are N-1 unknowns, $y^{1} \cdots\cdots y^{N-1}$. Treating J as any algebraic function to find the extremal, the necessary conditions according to Weierstrass' Theorem are:

$$\frac{\partial J}{\partial y^{i}} = 0 \quad ; \quad i = 1,2,\cdots\cdots N\text{-}1 \qquad \ldots.III\text{-}9$$

Solution of the N-1 algebraic equations III-9 should yield an approximation to the optimal function $y^{*}(t)$. Greenspan[2] considered a variety of problems with great success using this technique.

One immediately wonders why such a simple and direct approach has not received more attention. This can be attributed to two factors. Firstly, the equations defined by III-9 may be difficult to solve. A large number of algebraic (sometimes nonlinear) equations such as equation III-9 can only be solved on the modern high speed digital computer. Hence, when such methods were originally developed almost a century ago they could only be applied to the simpliest of problems. Secondly, there is no clear cut theory predicting when the sequence, y^{i}, will converge to the true minimum, $y^{*}(t)$. It must be remembered that this problem of convergence exists in most numerical procedures and often some experimentation with step size, Δt, may be necessary.

General Formulation of the Direct Finite Difference Method for Optimal Control Problems

A typical optimal control problem may be stated as follows. Consider the dynamic system defined in vector notation by:

$$\dot{\underline{x}} = \underline{F}(\underline{x},\underline{u},t) \qquad \text{....III-10}$$

subject to initial conditions:

$$\underline{x} = x_o \quad \text{at} \quad t = t_o \qquad \text{....III-11}$$

where: $\underline{x}$ is the state vector,

$\underline{u}$ is the control vector,

t is the time.

Find the control $\underline{u}(t)$ that minimizes the performance index

$$J = \int_o^{t_f} L(\underline{x},\underline{u},t)\ dt \qquad \text{....III-12}$$

To apply the direct finite difference method, we treat the system equations III-10 as constraints. Using Lagrange multipliers $\underline{\lambda}(t)$, we adjoin the system equations to the performance index to get a modified performance index:

$$K = \int_{t_o}^{t_f} \{L(\underline{x},\underline{u},t) + \underline{\lambda}^T [\underline{F}(\underline{x},\underline{u},t) - \dot{\underline{x}}]\} dt \qquad \text{....III-13}$$

where: $\underline{\lambda}^T$ is the transpose of $\underline{\lambda}$

Now the problem is to minimize K and is similar to problems in the calculus of variations. We divide the interval from t_o to t_f into N equal subintervals using the gridpoints $t_o, t_1, \cdots\cdots, t_{N-1}, t_f$. Corresponding

to these points we have values of the dependent variables:

$$\underline{x}^1, \underline{x}^2, \cdots\cdots, \underline{x}^N$$
$$\underline{u}^o, \underline{u}^1, \cdots\cdots, \underline{u}^{N-1}$$
$$\underline{\lambda}^o, \underline{\lambda}^1, \cdots\cdots, \underline{\lambda}^{N-1} \qquad \text{....III-14}$$

We approximate the integral K numerically by a series of rectangular strips using forward difference quotients for the derivatives.

$$\begin{aligned} K \cong & \{L(\underline{x}^o, \underline{u}^o, t_o) + \underline{\lambda}^{T^o}[\underline{F}(\underline{x}^o, \underline{u}^o, t_o) - \dot{\underline{x}}^o]\}\Delta t \\ & + \{L(\underline{x}^1, \underline{u}^1, t_1) + \underline{\lambda}^{T^1}[\underline{F}(\underline{x}^1, \underline{u}^1, t_1) - \dot{\underline{x}}^1]\}\Delta t \\ & \vdots \\ & + \{L(\underline{x}^{N-1}, \underline{u}^{N-1}, t_{N-1}) + \underline{\lambda}^{T^{N-1}}[\underline{F}(\underline{x}^{N-1}, \underline{u}^{N-1}, t_{N-1}) - \dot{\underline{x}}^{N-1}]\}\Delta t \end{aligned}$$

....III-15

If the system is of order k (i.e., $\underline{x}$ is a 1 by k vector), the total unknowns listed in equation III-14 are 3Nk. Hence, we need 3Nk equations to solve for these unknowns.

The required equations are obtained from the necessary conditions for an extremal as follows:

$$\frac{\partial K}{\partial \underline{x}^1} = 0, \quad \frac{\partial K}{\partial \underline{x}^2} = 0, \cdots\cdots, \frac{\partial K}{\partial \underline{x}^N} = 0 \quad \text{Nk equations} \qquad \text{....III-16}$$

$$\frac{\partial K}{\partial \underline{u}^o} = 0, \quad \frac{\partial K}{\partial \underline{u}^1} = 0, \cdots\cdots, \frac{\partial K}{\partial \underline{u}^{N-1}} = 0 \quad \text{Nk equations} \qquad \text{....III-17}$$

$$\frac{\partial K}{\partial \underline{\lambda}^o} = 0, \quad \frac{\partial K}{\partial \underline{\lambda}^1} = 0, \cdots\cdots, \frac{\partial K}{\partial \underline{\lambda}^{N-1}} = 0 \quad \text{Nk equations} \qquad \text{....III-18}$$

Solution of these 3Nk simultaneous algebraic equations will yield a possible optimal control sequence, $\underline{u}^o$, $\underline{u}^1$, ·····, $\underline{u}^{N-1}$ along with the optimal state trajectory and Lagrange multipliers. However, it should be remembered that equations III-16, III-17 and III-18 are only necessary conditions. Thus, the solution may be any stationary point and might even maximize K. The solution should be compared to other possible controls to establish whether it is optimal.

Example I: Application to a Simple Optimal Control Problem

The method is best understood by considering a simple example. Given the dynamical system described by the differential equation:

$$\frac{dx(t)}{dt} = -x(t) + u(t) \qquad \text{....III-19}$$

find the control, u(t), that minimizes the quadratic performance index:

$$J = \int_{t_o}^{t_f} [x(t)^2 + \rho u(t)^2]dt \qquad \text{....III-20}$$

In these equations, x(t) is the state variable, u(t) is the control variable, t is the time, and ρ is a constant. For this example, let

$t_o = 0.0$

$t_f = 1.0$

$\rho = 1.0$

$x = 2.0$ at $t = 0$

$x =$ unspecified at $t = t_f$

The final time is specified while the final state $x(t_f)$ is free.

The first step in the solution procedure is to treat the system differential equation (equation III-19) as a constraint and adjoin it to the performance index (equation III-20). This results in a modified performance index K:

$$K = \int_{t_o}^{t_f=1.0} \{x(t)^2+u(t)^2+\lambda(t)[-x(t)+u(t)-\frac{dx(t)}{dt}]\}dt \quad \ldots\ldots III\text{-}21$$

where $\lambda(t)$ is a Lagrangian multiplier. Now the problem is to find $x(t)$, $u(t)$, and $\lambda(t)$ such that K is minimized.

To solve the problem numerically we first divide the interval from t_o to t_f into N equal parts of length $\Delta t = \frac{t_f-t_o}{N}$. This division defines the grid points t_o, t_1, t_2, $\cdots\cdots$, t_{N-1}, t_f on the time axis and the corresponding values x^o, x^1, $\cdots\cdots$, x^N; u^o, u^1, $\cdots\cdots$, u^N; λ^o, λ^1, $\cdots\cdots$, λ^N, control and adjoint variables. We now approximate the integral K by means of a series of rectangular strips of width Δt using forward difference approximations for the derivatives appearing in K. The result is:

$$\begin{aligned} K \approx\ & \{(x^o)^2+(u^o)^2+\lambda^o[-x^o+u^o-(\frac{x^1-x^o}{\Delta t})]\}\Delta t \\ & + \{(x^1)^2+(u^1)^2+\lambda^1[-x^1+u^1-(\frac{x^2-x^o}{\Delta t})]\}\Delta t \\ & \vdots \\ & + \{(x^{N-1})^2+(u^{N-1})^2+\lambda^{N-1}[-x^{N-1}+u^{N-1}-(\frac{x^N-x^{N-1}}{\Delta t})]\}\Delta t \end{aligned} \quad \ldots\ldots III\text{-}22$$

K is an algebraic expression depending on the "variables" x^1, $\cdots\cdots$, x^N;

u^o, ..., u^{N-1}; λ^o, ...λ^{N-1}. The necessary conditions for an extremal are obtained by setting the partials of K with respect to each of these variables equal to zero:

$$\frac{\partial K}{\partial x^1} = 2x^1\Delta t - \lambda^o - \lambda^1\Delta t + \lambda^1 = 0$$

$$\frac{\partial K}{\partial x^2} = 2x^2\Delta t - \lambda^1 - \lambda^2\Delta t + \lambda^2 = 0$$

$$\frac{\partial K}{\partial x^{N-1}} = 2x^{N-1}\Delta t - \lambda^{N-2} - \lambda^{N-1}\Delta t + \lambda^{N-1} = 0$$

$$\frac{\partial K}{\partial x^N} = -\lambda^{N-1} = 0 \qquad \text{....III-23}$$

$$\frac{\partial K}{\partial u^o} = 2u^o\Delta t + \lambda^o\Delta t = 0$$

$$\frac{\partial K}{\partial u^1} = 2u^1\Delta t + \lambda^1\Delta t = 0$$

$$\frac{\partial K}{\partial u^{N-1}} = 2u^{N-1}\Delta t + \lambda^{N-1}\Delta t = 0 \qquad \text{....III-24}$$

$$\frac{\partial K}{\partial \lambda^o} = -x^o\Delta t + u^o\Delta t - x^1 + x^o = 0$$

$$\frac{\partial K}{\partial \lambda^1} = -x^1\Delta t + u^1\Delta t - x^2 + x^1 = 0$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = -x^{N-1}\Delta t + u^{N-1}\Delta t - x^N + x^{N-1} = 0 \qquad \text{....III-25}$$

Equations III-23, III-24 and III-25 are a set of 3N simultaneous linear algebraic equations which can be solved for the 3N unknowns: x^1, ...,x^N;

$u^o, \ldots\ldots, u^{N-1}; \lambda^o, \ldots\ldots, \lambda^{N-1}$.

The solution gives an approximation of a control u(t) which gives an extremal value of the performance index J. The smaller the time interval Δt the better this approximation will be. However, since equations III-23, III-24, and III-25 only guarantee an extremal value of J, there is no assurance that the calculated control u(t) will minimize J--it may in fact maximize J. This problem also usually exists in the maximum principle treatment of optimal control problems. The user must satisfy himself by further considerations that he does indeed have a minimum.

It should be noted that equations III-23, III-24 and III-25 are identical to a finite difference form of the differential equations obtained from the maximum principle treatment of the optimal control problem. Equations III-23, derived from $\frac{\partial K}{\partial x^i} = 0$, correspond to the finite difference form of the adjoint equations of the maximum principle. Equations III-25, derived from $\frac{\partial K}{\partial \lambda^i} = 0$, are just the original state equations. Equations III-24, derived from $\frac{\partial K}{\partial u^i} = 0$, are a finite difference form of $\frac{\partial H}{\partial u} = 0$ where H is the Hamiltonian function of maximum principle theory. This correspondence between the direct method and the maximum principle approach seems to hold true generally. In this sense, then, the direct method does not yield any new theory. It does provide an interesting alternative approach to obtaining the finite difference equations. It is felt that the direct method is worthy of further study in hopes that it may yield new insights into optimal control theory.

The above example of a first order linear system with quadratic

performance index was introduced to illustrate the direct method. The method will be applied in the same way to higher order systems, nonlinear systems, and other performance indices.

Solution of the Resulting Algebraic Equations

Equations III-23 through III-25 are typical of those obtained in the application of this method. For this reason, we will look more closely at this set of simultaneous equations.

Equations III-23 through III-25 may be written more conveniently in matrix-vector notation as follows:

$$\underline{A}\,\underline{X} + \underline{B} = 0 \qquad \text{....III-26}$$

where: $\underline{A}$ = n $\underline{x}$ n matrix of coefficients

$\underline{X}$ = n $\underline{x}$ 1 column vector of variables, $\underline{x}$, $\underline{u}$, $\underline{\lambda}$

$\underline{B}$ = n $\underline{x}$ 1 column vector of constants

To gain more insight into these equations, consider equations III-26 for n = 4.

$$\underline{A} = \begin{bmatrix}
2\Delta t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & (1-\Delta t) & 0 & 0 \\
0 & 2\Delta t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & (1-\Delta t) & 0 \\
0 & 0 & 2\Delta t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & (1-\Delta t) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 2\Delta t & 0 & 0 & 0 & \Delta t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2\Delta t & 0 & 0 & 0 & \Delta t & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2\Delta t & 0 & 0 & 0 & \Delta t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\Delta t & 0 & 0 & 0 & \Delta t \\
-1 & 0 & 0 & 0 & \Delta t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(1-\Delta t) & -1 & 0 & 0 & 0 & \Delta t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & (1-\Delta t) & -1 & 0 & 0 & 0 & \Delta t & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & (1-\Delta t) & -1 & 0 & 0 & 0 & \Delta t & 0 & 0 & 0 & 0
\end{bmatrix} \qquad \text{....III-27}$$

$$\underline{X} = \begin{bmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \\ u^o \\ u^1 \\ u^1 \\ u^3 \\ \lambda^o \\ \lambda^1 \\ \lambda^2 \\ \lambda^3 \end{bmatrix} \quad \text{....III-28} \qquad \underline{B} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ x^o(1-\Delta t) \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{....III-29}$$

Some observations are immediately apparent concerning the characteristic matrix, $\underline{A}$. Firstly, the matrix is large and "bulky". There are $(3N)^2$ elements for the first order system considered. Secondly, the matrix is "sparse", that is there are many zeros--in fact, most of the elements are zero. Thirdly, the nonzero elements are identical in diagonal sequences. These three properties are important when considering a method of solution.

In general, there are two approaches to solving linear simultaneous algebraic equations such as equation III-26--direct methods, such as Gauss and Gauss-Jordan eliminations, or indirect iterative procedures, such as Gauss-Seidel, and the generalized Newton method.[2,4,5]

For most problems encountered in engineering calculations, the direct methods are preferred because they require less computation time and give exact results in the absence of round-off errors. However, the particular properties of our characteristic matrix make these methods impractical; consequently, iterative procedures are preferred. The reasons for this are as follows:

(1) The direct methods require setting up the $\underline{A}$ matrix in core storage and then performing the elimination procedure. Even for the simple first order system, this requires $(3N)^2$ storage positions. Obviously, as N gets larger, the storage requirements of even the largest digital computers are insufficient.

(2) Round-off errors are significant when using direct methods. This is particularly true when the $\underline{A}$ matrix is large and sparse such as in our case.

(3) The system of equations is particularly easy to program for iterative procedures when the $\underline{A}$ matrix is sparse and has identical nonzero diagonals as is true in our case.

Greenspan[2] has successfully used a modified Newton-Raphson method (termed the "generalized Newton's method"). To illustrate this method, consider a set of j equations in j unknowns:

$$f_1(x_1,x_2,x_3, \cdots\cdots, x_j) = 0$$
$$f_2(x_1,x_2,x_3, \cdots\cdots, x_j) = 0$$
$$f_3(x_1,x_2,x_3, \cdots\cdots, x_j) = 0$$
$$f_j(x_1,x_2,x_3, \cdots\cdots, x_j) = 0 \qquad \text{....III-30}$$

The modified Newton-Raphson method solves these equations by an iterative procedure in which the value of an unknown for the n+1 iteration, x_i^{n+1}, is obtained from its value on the n^{th} iteration, x_i^n, by the following algorithm:

$$x_1^{n+1} = x_1^n - Z\{[f_1(x_1^n, x_2^n, x_3^n, \cdots\cdots, x_j^n)]/[\frac{\partial f_1(x_1^n, x_2^n, x_3^n, \cdots\cdots, x_j^n)}{\partial x_1}]\}$$

$$x_2^{n+1} = x_2^n - Z\{[f_2(x_1^{n+1}, x_2^n, x_3^n, \cdots\cdots, x_j^n)]/[\frac{\partial f_2(x_1^{n+1}, x_2^n, x_3^n, \cdots\cdots, x_j^n)}{\partial x_2}]\}$$

$$x_3^{n+1} = x_3^n - Z\{[f_3(x_1^{n+1}, x_2^{n+1}, x_3^n, \cdots\cdots, x_j^n)]/[\frac{\partial f_3(x_1^{n+1}, x_2^{n+1}, x_3^{n+1} \cdots\cdots, x_j^n)}{\partial x_3}]\}$$

$$x_j^{n+1} = x_j^n - Z\{[f_j(x_1^{n+1}, x_2^{n+1}, x_3^{n+1}, \cdots\cdots, x_j^n)]/[\frac{\partial f_j(x_1^{n+1}, x_2^{n+1}, x_3^{n+1}, \cdots\cdots, x_j^n)}{\partial x_j}]\}$$

The constant Z is a weighting factor that may be adjusted to help achieve convergence. Greenspan[2] recommends selecting Z in the range 0 to 2.

This algorithm is quite straightforward. Programming for large systems of equations of the kind encountered in the direct method is easy. Because of the sequential nature of the simultaneous equations III-23 through III-25, each equation need not be set up individually. The N equations (equation III-23) are all of the same general form and may be set up easily as a computer subroutine with a parameter running from 1 to N. The same is true for the N equations (equations III-24 and III-25). Thus, three simple algorithms can be set up to handle the 3N equations (equations III-23 through III-25) regardless of the size of N. Not only

does this lead to a simple program but the core storage required is small. There is no need to store all the coefficients of the matrix of the 3N equations. The coefficients are generated as needed by the three algorithms mentioned above.

Of course there are drawbacks to using this or any other iterative procedure. The major problem is convergence. For linear systems, this is not a great difficulty. The linear equations involved in this study all converged very quickly if the equations were arranged so that the coefficient of x_n in equation f_n was as large, or larger, in absolute value than the coefficients of the other variables in f_n. For nonlinear equations, however, convergence is a great problem. For the nonlinear equations in this study, some experimentation in first trial values and the weighting factor Z were necessary to obtain convergence. However, this was considered a small price to pay for the simplicity of the algorithm and the small amount of programming effort required. It is felt, provided the nonlinearities involved are not too severe, the method will be a useful one.

Returning to the original example problem, it is observed that good results are obtained even for a small number of increments, N.

Results of Example I

Solution of equations III-23 through III-25 was obtained for N = 5, 10, 20, and 50. The resulting control and state are compared to the true optimal. For this problem, the optimal control and state can be obtained analytically via the minimum principle as is done by Koppel[6].

The analytical results are:

$$u^*(t) = \frac{x(o)}{\beta} \sinh \alpha(t_f - t) \qquad \text{....III-31}$$

$$x^*(t) = \frac{x(o)}{\beta}[\alpha \cosh \alpha(t_f - t) + \sinh \alpha(t_f - t)] \qquad \text{....III-32}$$

where: $\alpha = \sqrt{1+p^{-1}}$

$\beta = \alpha \cosh \alpha(t_f - t_o) + \sinh \alpha(t_f - t_o)$

Figure III-1 compares the state trajectory for different numbers of increments to the optimal of equation III-32. Figure III-2 compares the controls. Note that as N increases the control and state converge to the optimal.

Percent deviation from the optimal is calculated by averaging deviations at three points (t = .2, .4, .6). This is shown as a function of N in Figure III-3. Note that for N = 20 less than 4% deviation from the optimal state trajectory and control is observed. For N = 50, a 0.448% deviation from optimal state trajectory and a 1.2% deviation from optimal control results.

It is interesting that for as few as ten increments (N = 10) an acceptable approximation to the optimal control results. The solution of the thirty linear algebraic equations presents no problems by the method discussed previously.

Other Numerical Approximations

A key step in the procedure is the numerical approximation of

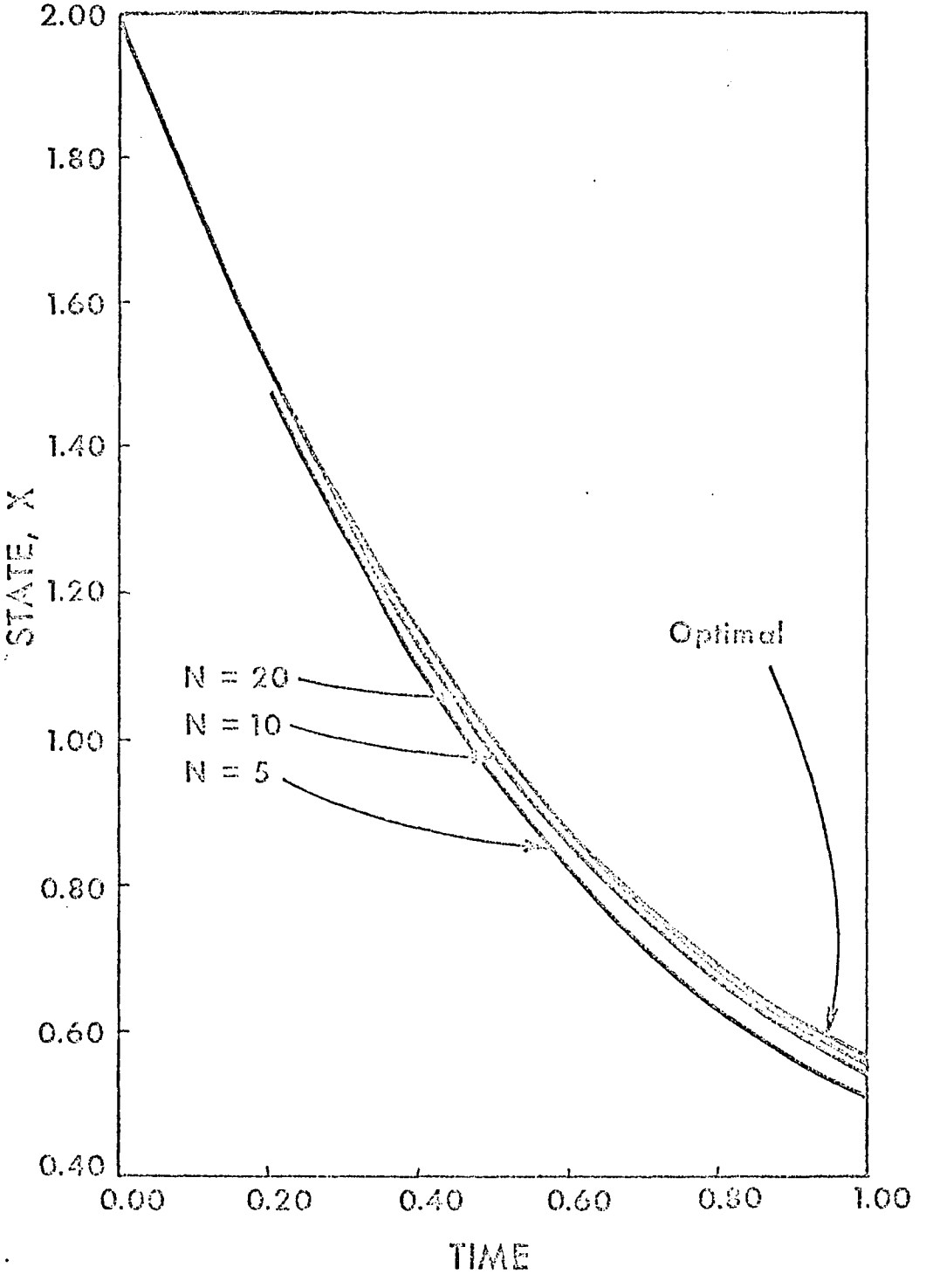

Figure III-1 Comparison of State Trajectories

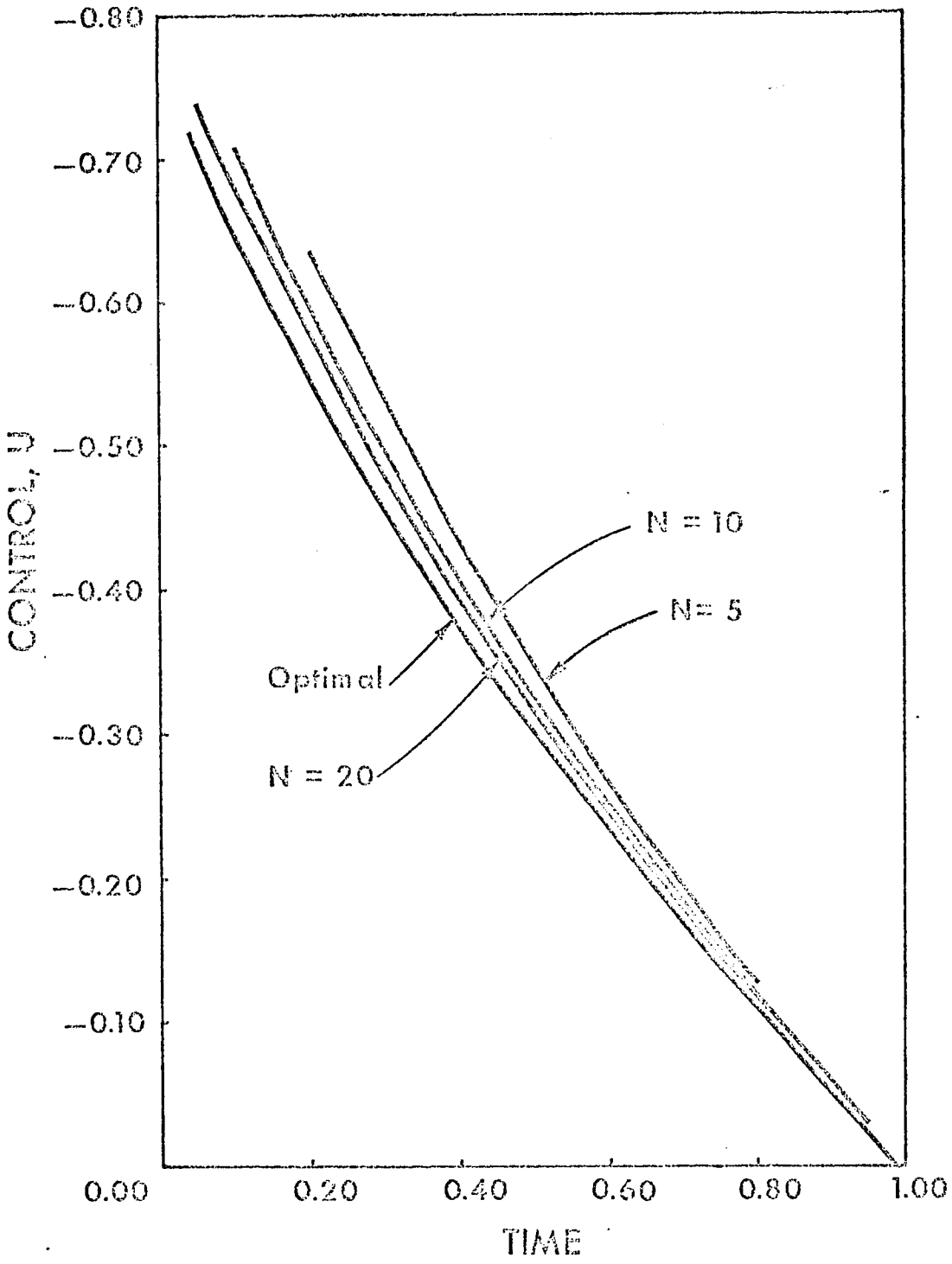

Figure III-2 Approximate and Optimal Control: U

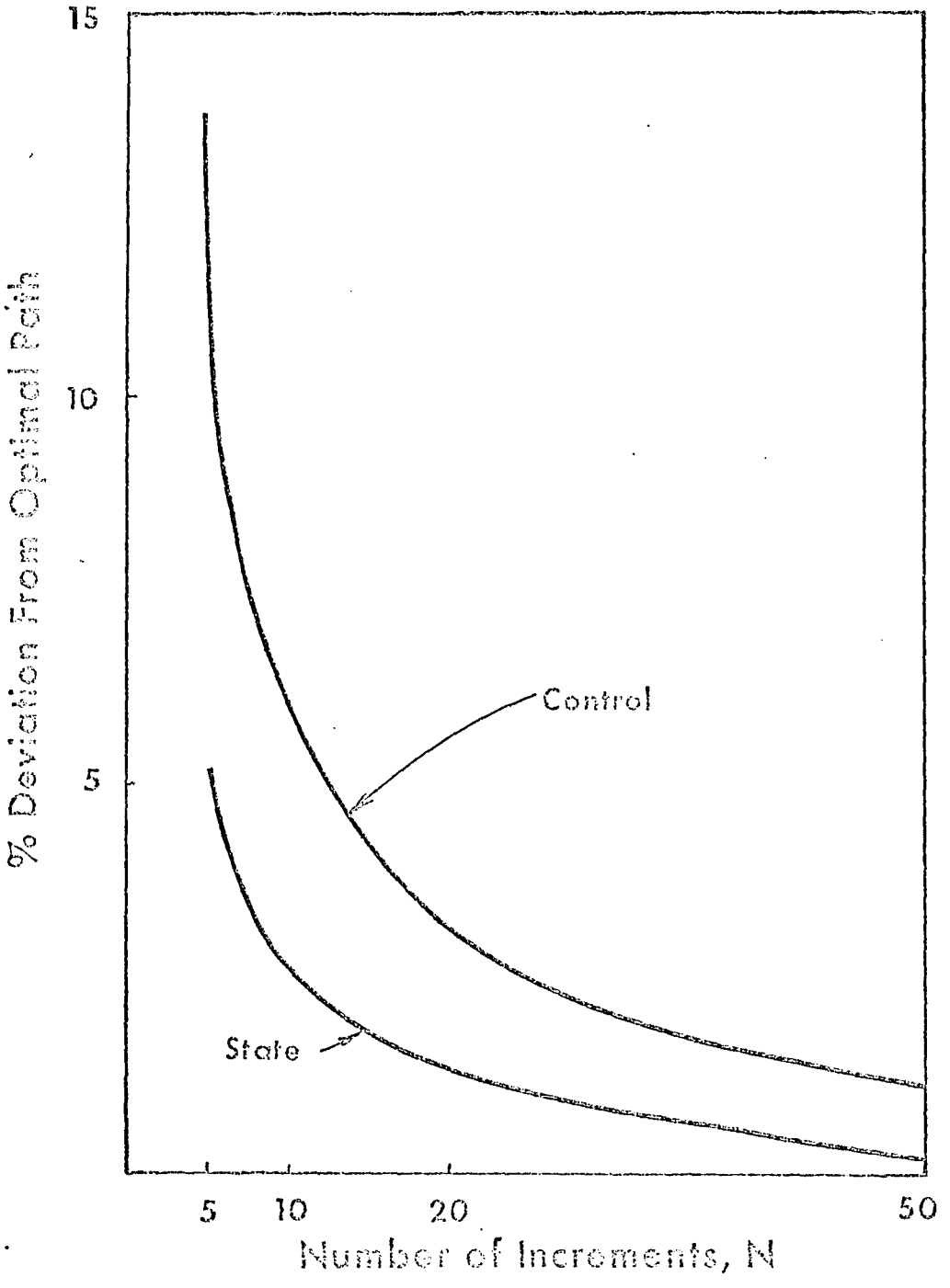

Figure III-3. Percent Deviation From Optimal versus Number of Increments

the adjoined performance index. This involves two approximations--the integral itself and the derivatives within this integral. In the previous examples the integral was approximated by N rectangles and the derivatives by forward differences.

An easy way to improve these approximations is to use a trapezoidal integration formula and a higher order, central difference approximation to the derivatives. Theoretically, even more sophisticated (higher order) numerical approximations could be used. However, for simplicity, we will be content to use these approximations.

The trapezoidal integration formula is defined by:

$$\int_a^b f(t)dt \cong \sum_{i=1}^{n} \frac{\Delta t}{2}[f(t_{i-1}) + f(t_i)]$$

$$\cong \frac{h}{2}[f(a) + 2f(a+\Delta t) + \cdots + 2f(a-i\Delta t) + \cdots + 2f(a+n\Delta t)$$

$$+ f(b)] \qquad \ldots\text{.III-33}$$

The error associated with this approximation is proportional to $(\Delta t)^2$ while the error associated with the rectangular integration is proportional to Δt.

The central difference approximation of a derivative is defined by:

$$(\frac{dx}{dt})^i \approx \frac{x^{i+1} - x^{i-1}}{2\Delta t} \qquad \ldots\text{.III-34}$$

The error associated with the central difference approximation is proportional to $(\Delta t)^2$ while that of the forward difference is proportional

to (Δt). This second order approximation may cause stability problems. Whenever the difference approximation of a derivative is of higher order than the original derivative, the solution contains extraneous solutions which are not related to the true solution. Instability arises when these extraneous solutions become large compared to the true solution.[7]

Note that the application of the central difference approximation at points $t = t_o$ and $t = t_f$ would require knowledge of x outside the interval (t_o, t_f). To circumvent this problem the forward difference formula is used on the first point, t_o, and the backward difference formula is used on the last point, t_f.

Application of these algorithms to equation III-21 yields the following numerical approximation:

$$
\begin{aligned}
K \approx\ & \{(x^o)^2 + (u^o)^2 + \lambda^o[-x^o + u^o - (\frac{x^1 - x^o}{\Delta t})]\}\frac{\Delta t}{2} \\
& + \{(x^1)^2 + (u^1)^2 + \lambda^1[-x^1 + u^1 - (\frac{x^2 - x^o}{2\Delta t})]\}\Delta t \\
& \vdots \\
& + \{(x^{N-1})^2 + (u^N)^2 + \lambda^{N-1}[-x^{N-1} + u^{N-1} - (\frac{x^N - x^{N-2}}{2\Delta t})]\}\Delta t \\
& + \{(x^N)^2 + (u^N)^2 + \lambda^N[-x^N + u^N - (\frac{x^N - x^{N-1}}{\Delta t})]\}\frac{\Delta t}{2}
\end{aligned}
\qquad \text{....III-35}
$$

This new approximation to K increases the variables involved by two. The new variables defined are u^N and λ^N. The two additional equations involved are obtained from $\frac{\partial K}{\partial u^N}$ and $\frac{\partial K}{\partial \lambda^N}$. The 3N+2 necessary

conditions for this case become:

$$\frac{\partial K}{\partial x^1} = \partial x^1 \Delta t + \lambda^o/2 + \lambda^1 \Delta t - \lambda^2/2 = 0$$

$$\frac{\partial K}{\partial x^{N-1}} = \partial x^{N-1} \Delta t + \lambda^{N-2} + \lambda^{N-1} - \lambda^N/2 = 0$$

$$\frac{\partial K}{\partial x^N} = x^N \Delta t + \lambda^{N-1}/2 + \lambda^N \Delta t + \lambda^N/2 = 0 \qquad \text{....III-36}$$

$$\frac{\partial K}{\partial x^o} = 2u^o - \lambda^o = 0$$

$$\frac{\partial K}{\partial u^N} = 2u^N - \lambda^N = 0 \qquad \text{....III-37}$$

$$\frac{\partial K}{\partial \lambda^o} = -x^o \Delta t + u^o \Delta t - x^1 + x^o = 0$$

$$\frac{\partial K}{\partial \lambda^1} = -x^1 \Delta t + u^1 \Delta t - \frac{1}{2}x^2 + \frac{1}{2}x^o = 0$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = -x^{N-1} \Delta t + u^{N-1} \Delta t - \frac{1}{2}x^N + \frac{1}{2}x^{N-2} = 0$$

$$\frac{\partial K}{\partial \lambda^N} = -x^N \Delta t + u^N \Delta t - x^N + x^{N-1} = 0 \qquad \text{....III-38}$$

These linear algebraic equations were solved for N = 10 and compared with the first numerical approximation. Table III-1 shows this comparison with the optimal state trajectory. Table III-2 compares the two approximations with the optimal control. From these tables, it is apparent that a better approximation is obtained using trapezoidal integration and central differences.

Recall that in this problem the final time, t_f, was fixed as part of the problem specification. Another common method of specification is to fix the final state, $\underline{x}(t_f)$ and leave the final time free. Our finite difference method can easily handle this type problem with some modification. The following example will illustrate the procedure.

Example II: First Order System with Final State Fixed, Final Time Free

Again consider the first order system described by the differential equation:

$$\frac{dx(t)}{dt} = -x(t) + u(t) \qquad \text{....III-39}$$

We shall specify the same performance index as considered in Example I.

$$J = \int_{t_o}^{t_f} [x^2(t) + \rho u^2(t)]dt \qquad \text{....III-40}$$

In this case, however, t_f is free and $x(t_f)$ is specified along with

Table III-1

Comparison of Numerical Approximations
With Optimal State Trajectory

Time	Optimal State	Approx.1*	Approx.2*
0.2	1.52	1.50	1.52
0.4	1.16	1.13	1.16
0.6	0.90	0.86	0.90
0.8	0.70	0.67	0.70

*Approx.1 = Rectangular integration + forward difference

Approx.2 = Trapezoidal integration + forward-central-backward difference.

Table III-2

Comparison of Numerical Approximations
With Optimal Control

Time	Optimal Control	Approx.1*	Approx.2*
0.2	-0.56	-0.49	-0.53
0.4	-0.38	-0.32	-0.37
0.6	-0.24	-0.18	-0.23
0.8	-0.11	-0.06	-0.11

*Approx.1 = Rectangular integration + forward difference

Approx.2 = Trapezoidal integration + forward-central-backward difference.

$x(t_o)$. Let

$$t_o = 0.0$$

$$t_f = \text{unspecified}$$

$$\rho = 1.0$$

$$x = 2.0 \text{ at } t = 0$$

$$x = 1.0 \text{ at } t = t_f$$

Again the first step is to adjoin the system equation to the performance index:

$$K = \int_{t_o=0}^{t_f=\text{free}} \{x^2(t)+u^2(t)+\lambda(t)[-x(t)+u(t)-\frac{dx(t)}{dt}]\}dt \quad \ldots.\text{III-41}$$

We may now approximate K numerically by dividing the interval t_o to t_f into N equal parts:

$$\begin{aligned} K \approx & \{(x^o)^2+(u^o)^2+\lambda^o[-x^o+u^o-(\frac{x^1-x^o}{\Delta t})]\}\Delta t \\ & + \{(x^1)^2+(u^1)^2+\lambda^1[-x^1+u^1-(\frac{x^2-x^1}{\Delta t})]\}\Delta t \\ & \vdots \\ & + \{(x^{N-1})^2+(u^{N-1})^2+\lambda^{N-1}[-x^{N-1}+u^{N-1}-(\frac{x^N-x^{N-1}}{\Delta t})]\}\Delta t \end{aligned} \quad \ldots.\text{III-42}$$

Note that although equations III-41 and III-21 look identical, there is a significant difference. In equation III-21, Δt is specified by the specification of N, t_o and t_f. In equation III-41, however, only

N and t_o are specified; hence, Δt is an unknown variable. Also the final value of x, x_N, is fixed. Therefore, we still have 3N unknowns.

We now treat equation III-41 as any algebraic equation with 3N unknowns and write the 3N necessary conditions for an external as follows:

$$\frac{\partial K}{\partial x^1} = 2x^1\Delta t - \lambda^o - \lambda^1\Delta t + \lambda^1 = 0$$

$$\frac{\partial K}{\partial x^2} = 2x^2\Delta t - \lambda^1 - \lambda^2\Delta t + \lambda^2 = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial x^{N-1}} = 2x^{N-1}\Delta t - \lambda^{N-2} - \lambda^{N-1}\Delta t + \lambda^{N-1} = 0 \qquad \text{....III-43}$$

$$\frac{\partial K}{\partial u^o} = 2u^o + \lambda^o = 0$$

$$\frac{\partial K}{\partial u^1} = 2u^1 + \lambda^1 = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial u^{N-1}} = 2u^{N-1} + \lambda^{N-1} = 0 \qquad \text{....III-44}$$

$$\frac{\partial K}{\partial \lambda^o} = -x^o \Delta t + u^o \Delta t - x^1 + x^o = 0$$

$$\frac{\partial K}{\partial \lambda^1} = -x^1 \Delta t + u^1 \Delta t - x^2 + x^1 = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = -x^{N-1} \Delta t + u^{N-1} \Delta t - x^N + x^{N-1} = 0 \qquad \text{....III-45}$$

$$\frac{\partial K}{\partial (\Delta t)} = (x^o)^2 + (u^o)^2 + \lambda^o(-x^o + u^o)$$

$$+ (x^1)^2 + (u^1)^2 + \lambda^1(-x^1 + u^1)$$

$$\vdots$$

$$+ (x^{N-1})^2 + (u^{N-1})^2 + \lambda^{N-1}(-x^{N-1} + u^{N-1}) = 0$$

....III-46

Observe that equations III-43 and III-45 are nonlinear since Δt is a variable. Also observe that we have omitted the partial of K with respect to x_N since x_N is a constant and that we treat Δt as any other variable in writing equation III-46.

Solution of these 2N nonlinear and N linear algebraic equations should yield our optimal control, state trajectory and value of Δt. The final time is calculated from:

$$t_f = N \Delta t \qquad \text{....III-47}$$

For this example, N was set equal to five and application of equations III-43 through III-46 resulted in fifteen equations and fifteen unknowns. Solution resulted in a Δt equal to 0.091 or a final time equal to 0.455. This compares favorably with an analytical final time of 0.467 obtained via the minimum principle. The optimal state and optimal control are compared to that obtained by solution of the algebraic equations in Figures III-4 and III-5. Also plotted in Figure III-5, is the optimal control obtained using trapezoidal integration with forward difference on the first point, central difference approximation in the center of the interval and backward difference on the last point. This is labeled Approximation 2. Note, once again, that improvement in the approximation is obtained.

We have considered two typical linear optimal control problems and have shown that a good approximation to the optimal control can be obtained using the direct finite difference method. It is significant that,even with a rather large step size,acceptable results were obtained.

This direct method can also be adapted to handle other types of optimal control problems. A problem frequently encountered is the case where the control is constrained and is required to drive the system from one point to another in minimum time. Such minimum time problems are of pratical importance in process control. For example, in processes which are subject to many set point changes, it may be desirable to design a control algorithm in order to accomplish this as

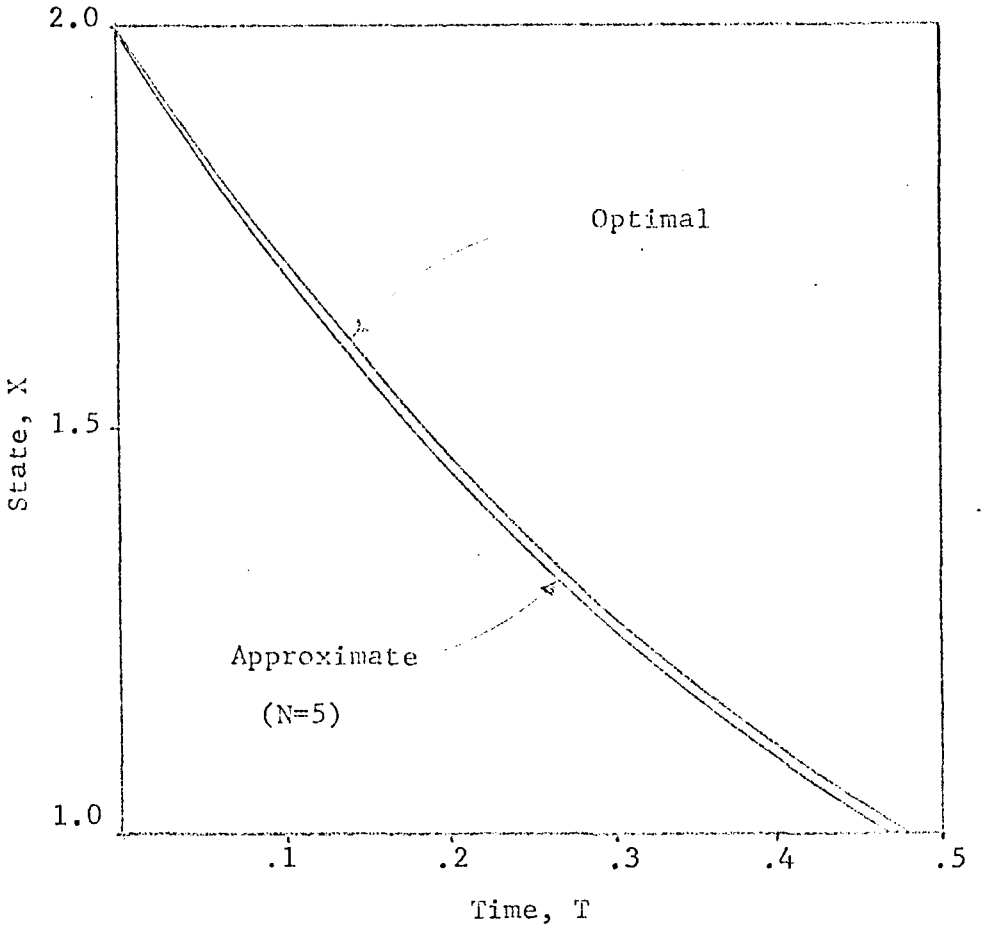

Figure III-4

Optimal and Approximate State Trajectories
For Final State Specified (Example II)

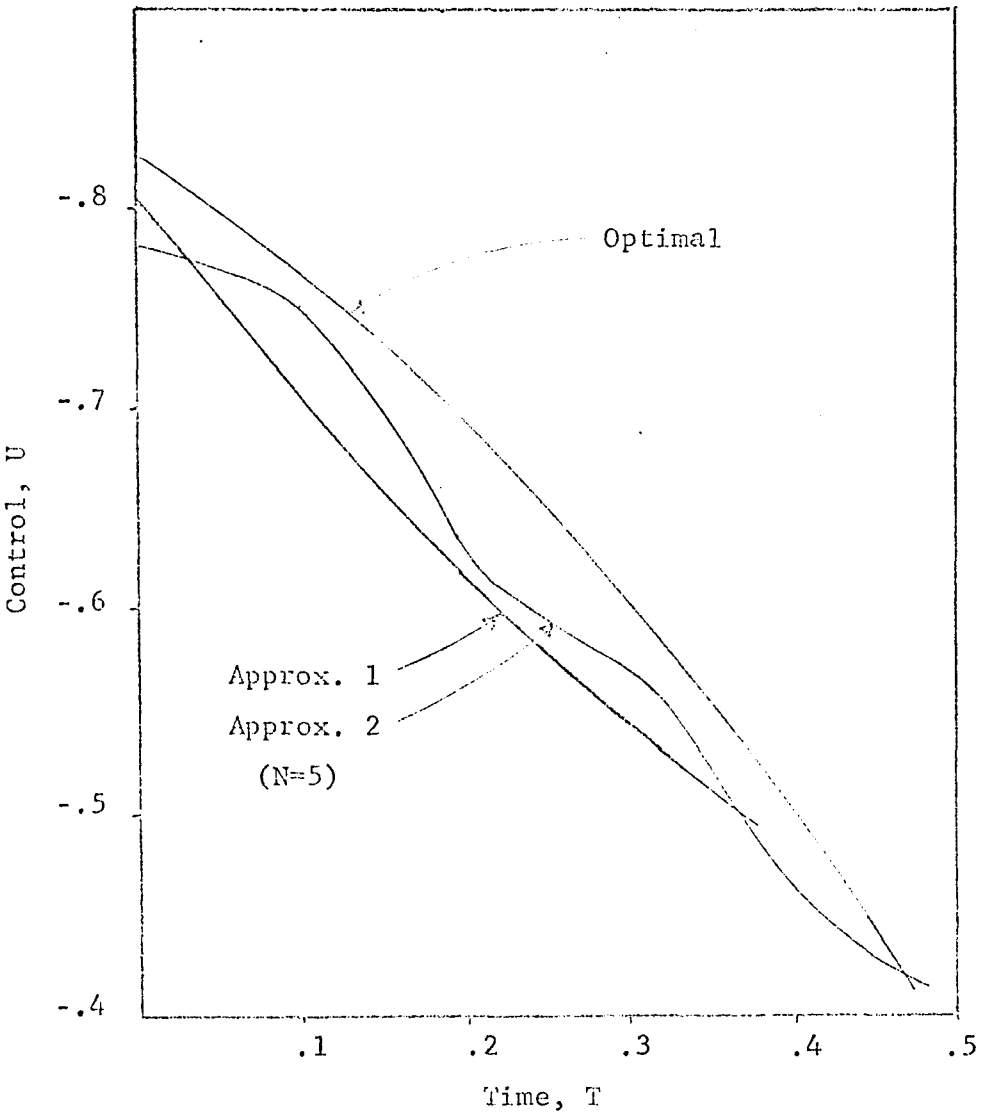

Figure III-5

Optimal and Approximate Control for Example II

Approx. 1 = Forward Differences and Rectangular Integration
Approx. 2 = Forward-Central-Backward Differences and Trapezoidal Integration

rapidly as possible. Also, there is usually a physical limit, such as the size of a valve, set upon the control action. To illustrate application of the direct procedure to the minimum time or time optimal control problem, a simple linear example follows.

Example III: Time Optimal Control via the Direct Method

Consider the second order system defined by the following differential equation:

$$\frac{d^2x}{dt^2} = u \qquad \text{....III-48}$$

This is termed the double integral plant by Athans[8] who outlines the analytical solution for such problems.

It is desired to drive the system from x=1 initially to x=0 in minimum time. The final time, t_f, that is to be minimized is not specified. The initial and final value of the first derivatives are specified as:

$$(\frac{dx}{dt}) = 1 \qquad \text{at } t = 0$$

$$(\frac{dx}{dt}) = 0 \qquad \text{at } t = 0$$

The control is constrained by:

$$|u| \leq 1.0 \qquad \text{....III-49}$$

The performance index may be written as:

$$J = t_f = \int_o^{t_f} dt \qquad \text{....III-50}$$

Optimal control theory specifies that for a linear second order system, such as equation III-48, and performance index, such as equation III-50, the control will be bang-bang with, at most, one switch from minimum to maximum value of u (or vice versa). This fact will be utilized to set up our direct algorithm in a modified form.

Equation III-48 can be redefined in state variable form as follows:

$$x_1 = x \qquad \text{....III-51}$$

$$\dot{x}_1 = x_2 \qquad \text{....III-52}$$

$$\dot{x}_2 = u \qquad \text{....III-53}$$

The boundary conditions can now be written as:

$$x_1(t_o) = 1$$
$$x_1(t_f) = 0$$
$$x_2(t_o) = 1$$
$$x_2(t_f) = 0$$

Assuming that the control starts at the maximum value, u_{max}, and switches to its minimum value, u_{min}, at the switching time, t_s, the problem is now to find the switching time and determine if this

sequence of switching is optimal.

Adjoining the system equations III-52 and III-53 to the performance index results in:

$$K = \int_o^{t_f} [1 + \lambda_1(x_2 - \dot{x}_1) + \lambda_2(u - \dot{x}_2)]dt \qquad \text{....III-54}$$

We have, however, assumed that u is equal to u_{min} from 0 to t_s and u_{max} from t_s to t_f. Therefore, u is not an unknown and may be replaced by its appropriate value. To do this, we divide the interval into two parts:

$$K = \int_o^{t_s} [1 + \lambda_1(x_2 - \dot{x}_1) + \lambda_2(u_{min} - \dot{x}_2)]dt + \int_{t_s}^{t_f} [1 + \lambda_1(x_2 - \dot{x}_1) + \lambda_2(u_{max} - \dot{x}_2)]dt \qquad \text{....III-55}$$

We may now approximate each part of K numerically. This is done using rectangular integration and forward differences by dividing the interval 0 to t_s into N increments and the interval t_s to t_f into M increments:

$$\begin{aligned}
K \approx\ & \{1+\lambda_1^o[x_2^o - (\frac{x_1^1 - x_1^o}{\Delta t_1})] + \lambda_2^o[u_{min} - (\frac{x_2^1 - x_2^o}{\Delta t_1})]\}\Delta t_1 \\
& + \vdots \\
& + \{1+\lambda_1^{N-1}[x_2^{N-1} - (\frac{x_1^N - x_1^{N-1}}{\Delta t_1})] + \lambda_2^{N-1}[u_{min} - (\frac{x_2^N - x_2^{N-1}}{\Delta t_1})]\}\Delta t_1 \\
& + \{1+\lambda_1^N[x_2^N - (\frac{x_1^{N+1} - x_1^N}{\Delta t_2})] + \lambda_2^N[u_{max} - (\frac{x_2^{N+1} - x_2^N}{\Delta t_2})]\}\Delta t_2 \\
& \vdots \\
& + \{1+\lambda_1^{N+M-1}[x_2^{N+M-1} - (\frac{x_1^{N+M} - x_1^{N+M-1}}{\Delta t_2})] + \lambda_2^{N+M-1}[u_{max} - (\frac{x_2^{N+M} - x_2^{N+M-1}}{\Delta t_2})]\}\Delta t_2
\end{aligned} \qquad \text{....III-56}$$

where: $\Delta t_1 = \text{unknown} = \dfrac{t_s}{N}$

$$\Delta t_2 = \text{unknown} = \frac{t_f - t_s}{M}$$

Observe that Δt_1 and Δt_2 are unknowns and that by determining these we also determine t_s and t_f since N and M are specified as are x_1^o, x_1^{N+M}, x_2^o, and x_2^{N+M}. Hence, equation III-56 involves 4(N+M) unknowns as is tabulated in Table III-3.

The 4(N+M) necessary conditions are obtained as before by treating K as an algebraic expression. These are:

$$\frac{\partial K}{\partial x_1^1} = \lambda_1^o - \lambda_1^1 = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial x_1^{N+M}} = \lambda_1^{N+M-1} - \lambda_1^{N+M} = 0 \qquad \text{....III-57}$$

$$\frac{\partial K}{\partial x_2^1} = \lambda_2^o - \lambda_1^1 \Delta t_1 - \lambda_2^1 = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial x_2^{N-1}} = \lambda_2^{N-2} - \lambda_1^{N-1} \Delta t_1 - \lambda_2^{N-1} = 0$$

$$\frac{\partial K}{\partial x_2^N} = \lambda_2^{N-1} - \lambda_1^N \Delta t_2 - \lambda_2^N = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial x_2^{N+M-1}} = \lambda_2^{N+M-2} - \lambda_1^{N+M-1} \Delta t_2 - \lambda_2^{N+M-1} = 0 \qquad \text{....III-58}$$

$$\frac{\partial K}{\partial \lambda_1^o} = x_2^o - \left(\frac{x_1^1 - x_1^o}{\Delta t_1}\right) = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial \lambda_1^{N-1}} = x_2^{N-1} - \left(\frac{x_1^N - x_1^{N-1}}{\Delta t_1}\right) = 0$$

$$\frac{\partial K}{\partial \lambda_1^N} = x_2^N - \left(\frac{x_1^{N+1} - x_1^N}{\Delta t_2}\right) = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial \lambda_1^{N+M-1}} = x_2^{N+M-1} - \left(\frac{x_1^{N+M} - x_1^{N+M-1}}{\Delta t_2}\right) = 0 \qquad \text{....III-59}$$

$$\frac{\partial K}{\partial \lambda_2^o} = u_{min} - \left(\frac{x_2^1 - x_2^o}{\Delta t_2}\right) = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial \lambda_2^{N-1}} = u_{min} - \left(\frac{x_2^N - x_2^{N-1}}{\Delta t_1}\right) = 0$$

$$\frac{\partial K}{\partial \lambda_2^N} = u_{max} - \left(\frac{x_2^{N+1} - x_2^N}{\Delta t_2}\right) = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial \lambda_2^{N+M-1}} = u_{max} - \left(\frac{x_2^{N+M} - x_2^{N+M-1}}{\Delta t_2}\right) = 0 \qquad \text{....III-60}$$

$$\frac{\partial K}{\partial (\Delta t_2)} = 1 + \lambda_1^o x_2^o + \lambda_2^o u_{min}, + \ldots + , 1 + \lambda_1^{N-1} x_2^{N-1} + \lambda_2^{N-1} u_{min} = 0$$

....III-61

$$\frac{\partial K}{\partial(\Delta t_2)} = 1 + \lambda_1^N x_2^N + \lambda_2^N u_{max}, + \ldots. + 1 + \lambda_1^{N+M-1} x_2^{N+M-1} + \lambda_2^{N+M} u_{max} = 0$$

....III-64

Equations III-57 through III-62 may be simplified by noting that the N+M equations III-57 result in λ_1 = constant and may be dropped. This allows replacement of λ_1^o .... λ_1^{N+M-1} by a constant in equations III-58, III-61 and III-62. Our original 4(N+M) equations are now reduced to 3(N+M) + 1 algebraic equations.

These equations were solved for N = M = 6 and the results compared to the optimal solutions from Athans and Falb[8]. Figure III-6 illustrates the results. Again we see that even using a large step size, we obtain a good approximation to the optimal control.

It should be noted that to determine if our switching sequence is optimal, other possibilities should be assumed such as u_{max} from t_o to t_s and u_{min} from t_s to t_f. For a discussion of this, see Athans and Falb[8]. This could easily be done by replacing the values of u_{max} and u_{min} in equations III-60 and III-61. This will not be done now since we know that the correct switching sequence was assumed.

We have now considered three typical optimal control problems and illustrated how the finite difference method may be applied. All three were linear stationary autonomous systems. Systems with time varying coefficients can be handled in a "natural" way using the finite difference method. This will be illustrated by the following example.

Table III-3

Tabulation of Unknowns for Time Optimal Problem

Variable	Number of Unknowns
$x_1^1 - x_1^{N+M-1}$	N+M-1
$x_2^1 - x_2^{N+M-1}$	N+M-1
$\lambda_1^o - \lambda_1^{N+M-1}$	N+M
$\lambda_2^o - \lambda_2^{N+M-1}$	N+M
Δt_1	1
Δt_2	1
	Total = 4(N+M)

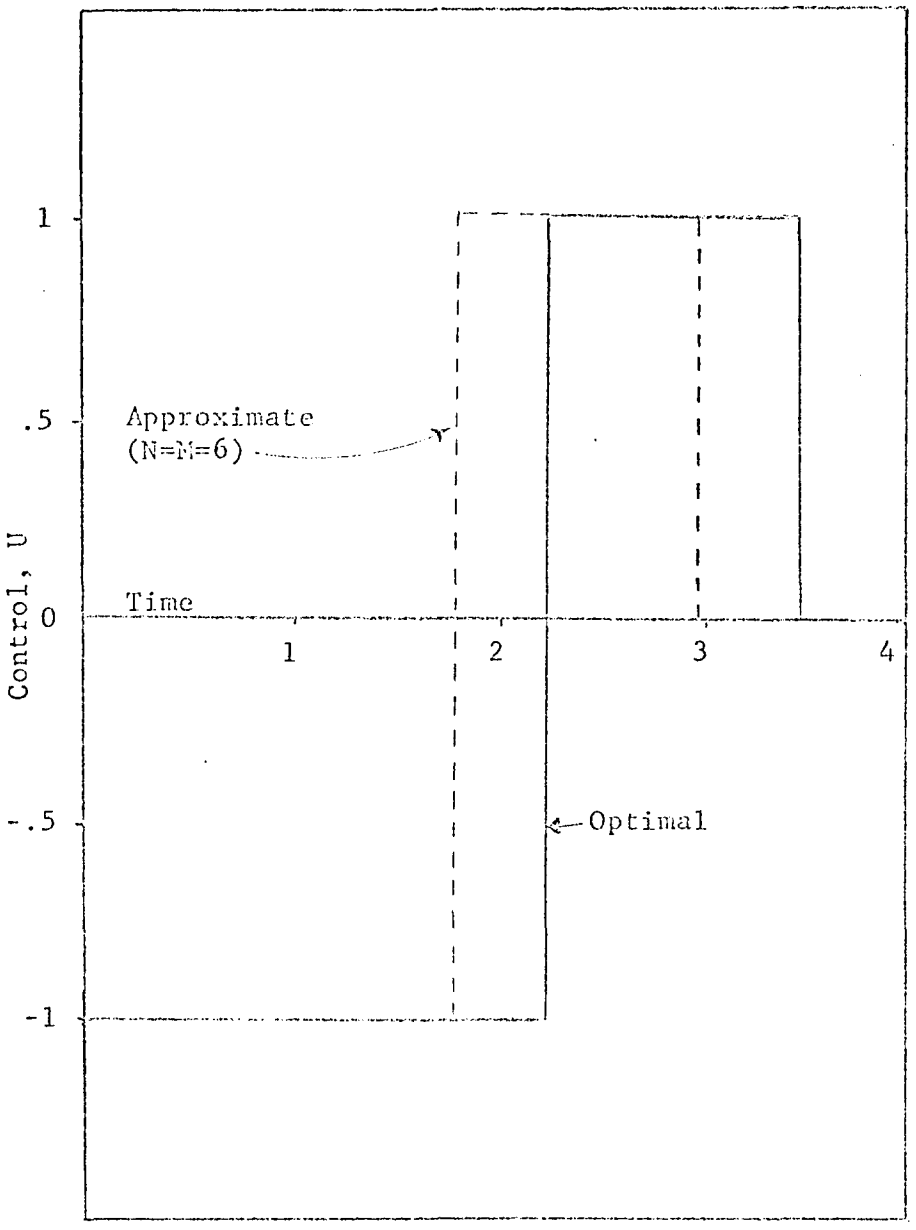

Figure III-6

Optimal and Approximate Minimum
Time Control

Example IV: Nonautonomous System

Consider the first order system defined by:

$$\frac{dx(t)}{dt} = c\ e^{pt}\ u(t) \qquad \text{....III-63}$$

where: c = constant

p = constant

The system is to be driven from $x(t_o) = 0$ to $x(t_f) = 2$, where t_f is specified as 2, in such a way as to minimize the control effort defined by:

$$J = \int_o^{t_f} u(t)^2 dt \qquad \text{....III-64}$$

This is termed a minimum fuel problem. Again, the first step is to adjoin our system equation to the performance index:

$$J = \int_o^{t_f} \{u(t)^2 + \lambda(t)[c\ e^{pt}\ u(t) - \frac{dx}{dt}]\}dt \qquad \text{....III-65}$$

Next, approximate J numerically. For this example, use trapezoidal integration with forward, central and backward approximations of the derivatives:

$$\begin{aligned} K \approx & \{(u^o)^2 + \lambda^o[ce^{pt_o}\ u^o - (\frac{x^1-x^o}{\Delta t})]\}\frac{\Delta t}{2} \\ & + \{(u^1)^2 + \lambda^1[ce^{pt_1}\ u^1 - (\frac{x^2-x^o}{2\Delta t})]\}\Delta t \\ & \vdots \\ & + \{(u^{N-1})^2 + \lambda^{N-1}[ce^{pt_{N-1}}\ u^{N-1} - (\frac{x^N-x^{N-2}}{2\Delta t})]\}\Delta t \\ & + \{(u^N)^2 + \lambda^N[ce^{pt_N}\ u^N - (\frac{x^N-x^{N-1}}{\Delta t})]\}\frac{\Delta t}{2} \end{aligned} \qquad \text{....III-66}$$

where: $t_n = n\ \Delta t$

$$\Delta t = \frac{t_f - t_o}{N} = \frac{2}{N}$$

$$x_o = 0$$

$$x_N = 2$$

Writing the necessary conditions for minimization of K yields:

$$\frac{\partial K}{\partial x^1} = -\lambda^o + \lambda^2 = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial x^{N-1}} = -\lambda^{N-2} + \lambda^N = 0 \qquad \text{....III-67}$$

$$\frac{\partial K}{\partial u^o} = 2u^o + \lambda^o c e^{pt_o} \frac{\Delta t}{2} = 0$$

$$\frac{\partial K}{\partial u^1} = 2u^1 + \lambda^1 c e^{pt_1} \frac{\Delta t}{2} = 0$$

$$\vdots$$

$$\frac{\partial K}{\partial u^{N-1}} = 2u^{N-1} + \lambda^{N-1} c e^{pt_{N-1}} \Delta t = 0$$

$$\frac{\partial K}{\partial u^N} = 2u^N + \lambda^N c e^{pt_N} \frac{\Delta t}{2} = 0 \qquad \text{....III-68}$$

$$\frac{\partial K}{\partial \lambda^o} = -x^1 + x^o + ce^{pt_o} u^o \Delta t = 0$$

$$\frac{\partial K}{\partial \lambda^1} = -x^2 + x^o + ce^{pt_1} u^1 \Delta t = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = -x^N + x^{N-2} + ce^{pt_{N-1}} u^{N-1} \Delta t = 0$$

$$\frac{\partial K}{\partial \lambda^N} = -x^N + x^{N-1} + ce^{pt_N} u^N \Delta t = 0 \qquad \text{....III-69}$$

The resulting 3(N+1) linear algebraic equations are easily solved. Solutions are presented for N = 5 and N = 10. The analytical solution to this problem, as presented in Fan [9] is:

$$u(t) = \frac{4p}{C(\exp(4p)-1)e^{pt}}$$

$$x(t) = \frac{2(\exp(2pt)-1)}{e^{4p}-1}$$

Figure III-7 compares the optimal and approximate control. Due to the wide range of values, the state trajectories are compared with optimal in Table III-4. Again, we see that even using relatively large step sizes, a good approximation to the optimal control is obtained.

Thus far, we have considered four rather simple examples to illustrate application of the direct finite difference method. A more complex problem involves the design of a multivariable optimal control

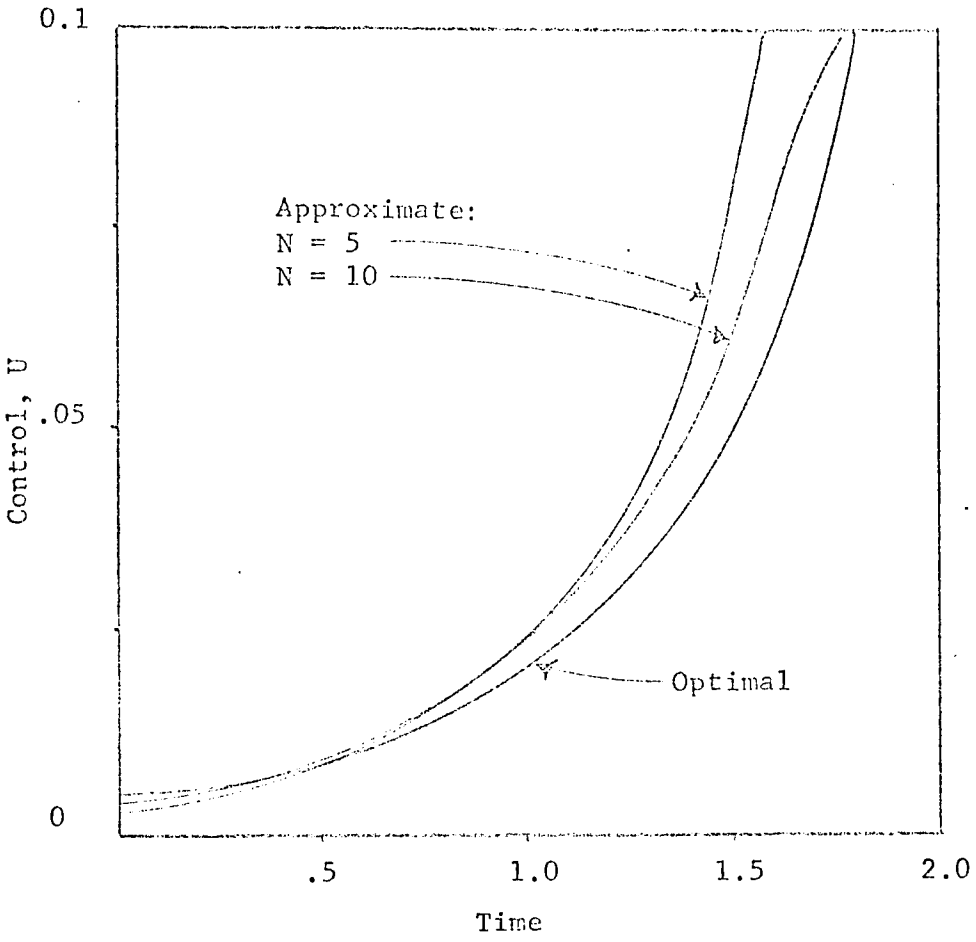

Figure III-7

Optimal and Approximate Control for Nonautonomous System

Table III-4

Comparison of Approximate and Optimal State Trajectories For Nonautonomous System

Time	State Trajectory		
	Optimal	N = 5	N = 10
0	0	0	0
.2	.0008	---	.0003
.4	.0027	.0008	.0027
.6	.0067	---	.0069
.8	.0158	.0114	.0158
1.0	.0360	---	.0397
1.2	.0809	.0791	.0809
1.4	.1808	---	.2019
1.6	.4033	.290	.4033
1.8	.8983	---	1.005
2.0	2.000	2.0	2.000

strategy. The system to be considered is a linearized backmix chemical reactor.

Example V: Linearized Stirred Tank Reactor Problem

The stirred tank reactor to be studied is shown in Figure III-8. It is the same system studied by Smith[10]. The problem is to control the outlet temperature T and the outlet concentration C_A at some desired set points, $\bar{T}$ and $\bar{C}_A$, in such a way as to minimize a specified cost function. The manipulated variables are the feed rate, w, and the heat added or removed, Q. In practice, not Q but the flow rate of cooling water through a jacket or cooling coils would be manipulated. This is related to Q through an unsteady state energy balance. For this problem, however, it is simpler to assume Q is directly manipulated and that enough heat transfer is available so that saturation does not occur. A large Q will be penalized in the cost function to ensure that too great a control effort will not occur. The system is driven by the initial conditions specified for temperature and concentration. This is the state regulator problem described by Athans and Falb[8] and physically may be interpreted as a "start-up" problem.

A second order irreversible reaction of the form

$$2A \rightarrow B$$

is assumed. The rate of reaction is expressed by:

$$\text{Rate} = kC_A^2 \qquad \ldots.\text{III-70}$$

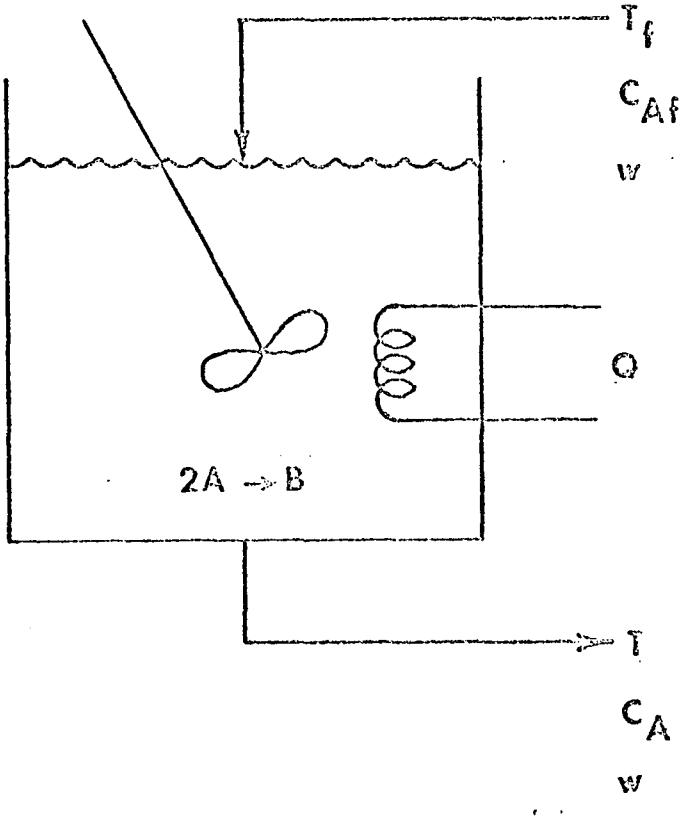

Figure III-8 Continuous Stirred-Tank Reactor

where the rate constant k is related to the temperature by an Arrhenius expression:

$$k = k_o \exp(-A/T) \qquad \text{....III-71}$$

It can be seen that the reaction rate is nonlinear both with respect to concentration and with respect to temperature.

Unsteady state material and energy balances on the reactor yield:

$$\frac{w}{V\rho}(C_{Af}-C_A) - kC_A^2 = \frac{dC_A}{dt} \qquad \text{....III-72}$$

$$\frac{w}{V\rho}(T_f-T) + \frac{Q}{V\rho C_p} - \frac{\Delta H k C_A^2}{\rho C_p} = \frac{dT}{dt} \qquad \text{....III-73}$$

In these equations, V is the reactor volume, ρ is the density of the reactor contents, C_p is the specific heat of the reactor contents, ΔH is the enthalpy change for the reaction, and t is the time. T_f and C_{Af} are the temperature and concentration of the feed.

Linearization of equations III-72 and III-73 about steady state or set point conditions yields:

$$\frac{d\hat{C}_A}{dt} = \left(-\frac{\hat{w}}{V\rho} - 2\bar{C}_A\bar{k}\right)\hat{C}_A - \left(\frac{\bar{k}A\bar{C}_A^2}{\bar{T}^2}\right)\hat{T} + \left(\frac{C_{Af}-\bar{C}_A}{V\rho}\right)$$

....III-74

$$\frac{d\hat{T}}{dt} = \left(\frac{-2\Delta H\bar{k}\bar{C}_A}{\rho C_p}\right)\hat{C}_A - \left[\frac{\bar{w}}{V\rho} + \left(\frac{\Delta H\bar{k}\bar{C}_A^2}{\rho\bar{T}^2C_p}\right)\right]\hat{T} + \frac{\hat{Q}}{V\rho C_p} + \left(\frac{T_f-\bar{T}}{V\rho}\right)\hat{w} \quad \ldots.\text{III-75}$$

The steady state values $\bar{C}_A$, $\bar{T}$, $\bar{Q}$, $\bar{w}$ and $\bar{k}$ are obtained from the steady state versions of equations III-72 and III-73. The variables $\hat{C}_A$, $\hat{T}$, $\hat{Q}$, and $\hat{w}$ are defined as variations about the steady state values; e.g., $\hat{C}_A = C_A - \bar{C}_A$.

For this example the following reactor parameters were chosen:

$$V = 13.38 \text{ ft}^3$$

$$\rho = 55 \text{ lb/ft}^3$$

$$C_p = 1.0 \text{ Btu/lb}^\circ\text{F}$$

$$\Delta H = -12000 \text{ Btu}$$

$$A = 14000^\circ\text{R}$$

$$k_o = 8.33 \times 10^8 \text{ ft}^3\text{/lb mole min}$$

$$T_f = 100^\circ\text{F}$$

$$C_{Af} = 0.4 \text{ lb moles/ft}^3$$

$$\bar{T} = 200^\circ\text{F}$$

$$\bar{C}_A = 0.2 \text{ lb moles/ft}^3$$

Solution of the steady state equations for these conditions yields steady state flow rate, rate constant, and heat duty as

$$\bar{w} = 75.2 \text{ lb/min}$$

$$\bar{k} = 0.51 \text{ ft}^3\text{/lb mole min}$$

$$\bar{Q} = 4238 \text{ Btu/min}$$

With these parameters the linearized equations may be written in matrix form as:

$$\dot{\underline{x}} = \underline{A}\,\underline{x} + \underline{B}\,\underline{u}$$

or

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \text{....III-76}$$

where the state variables are defined to be $x_1 = \hat{C}_A$, $x_2 = \hat{T}$, and the control variables are $\hat{u}_1 = w$ and $u_2 = \hat{Q}$. The matrix elements are:

$$\begin{aligned} a_{11} &= 0.041 & a_{12} &= 44.6 \\ a_{21} &= -0.001 & a_{22} &= -0.307 \\ b_{11} &= 0.001 & b_{12} &= -0.136 \\ b_{22} &= 0 & b_{22} &= 0.001 \end{aligned} \quad \text{....III-77}$$

The control variables $u_1(t)$ and $u_2(t)$ are to be chosen to minimize a quadratic cost index defined by:

$$J = \int_{t_o}^{t_f} [q_{11}x_1(t)^2 + q_{22}x_2(t)^2 + r_{11}u_1(t)^2 + r_{22}u_2(t)^2]dt \quad \text{....III-78}$$

with

$$\begin{aligned} q_{11} &= 0.1 & r_{11} &= 1.0 \\ q_{22} &= 1.0 & r_{22} &= 400 \end{aligned} \quad \text{....III-79}$$

Other parameters were set as follows:

$$t_o = 0 \qquad t_f = 1.0 \text{ min}$$

$$x_1^o = 20^oF \qquad x_2^o = 0.5 \text{ moles/ft}^3 \qquad \text{....III-80}$$

To solve by the direct finite difference method,we first adjoin the system equations to the performance index using the Lagrangian multipliers $\lambda_1(t)$ and $\lambda_2(t)$. This yields a new performance index K:

$$K = \int_o^{t_f} \{q_{11}x_1(t)^2 + q_{22}x_2(t)^2 + r_{11}u_1(t)^2 + r_{22}u_2(t)^2$$

$$+ \lambda_1(t)[a_{11}x_1 + a_{12}x_2 + b_{11}u_1 + b_{12}u_2 - \frac{dx_1}{dt}]$$

$$+ \lambda_2(t)[a_{21}x_1 + a_{22}x_2 + b_{21}u_1 + b_{22}u_2 - \frac{dx_2}{dt}]\}dt \qquad \text{....III-81}$$

K is then approximated numerically using "rectangular" integration and forward difference approximations for the derivatives. The resulting expression involves 6N independent variables where N is the number of intervals used between t_o and t_f. The 6N necessary conditions for an extremal are:

$$\frac{\partial K}{\partial x_1^1} = 2q_{11}x_1^1 + \lambda_1^1 a_{11}\Delta t + \lambda_2^1 a_{21}\Delta t + \lambda_1^1 - \lambda_1^o = 0$$

$$\frac{\partial K}{\partial x_1^{N-1}} = 2q_{11}x_1^{N-1} + \lambda_1^{N-1} a_{11}\Delta t + \lambda_2^{N-1} a_{21}\Delta t + \lambda_1^{N-1} - \lambda_1^{N-2} = 0$$

$$\frac{\partial K}{\partial x_1^N} = \lambda_1^N = 0$$

$$\frac{\partial K}{\partial x_2^1} = 2q_{22}x_2^1\Delta t + \lambda_2^1 a_{22}\Delta t + \lambda_1^1 a_{12}\Delta t + \lambda_2^1 - \lambda_2^o = 0 \qquad \text{....III-82}$$

$$\frac{\partial K}{\partial x_2^{N-1}} = 2q_{22}x_2^{N-1}\Delta t + \lambda_2^{N-1} a_{22}\Delta t + \lambda_1^{N-1} a_{12}\Delta t + \lambda_2^{N-1} - \lambda_2^{N-2} = 0$$

$$\frac{\partial K}{\partial x_2^N} = \lambda_2^N = 0 \qquad \text{....III-83}$$

$$\frac{\partial K}{\partial u_1^o} = 2r_{11}u_1^o + \lambda_1^o b_{11} = 0$$

$$\frac{\partial K}{\partial u_1^{N-1}} = 2r_{11}u_1^{N-1} - \lambda_2^{N-1} b_{11} = 0 \qquad \text{....III-84}$$

$$\frac{\partial K}{\partial u_2^o} = 2r_{22}u_2^o + \lambda_1^o b_{12} + \lambda_2^o b_{22} = 0$$

$$\frac{\partial K}{\partial u_2^{N-1}} = 2r_{22}u_2^{N-1} + \lambda_1^{N-1} b_{12} + \lambda_2^{N-1} b_{22} = 0 \qquad \text{....III-85}$$

$$\frac{\partial K}{\partial \lambda_1^o} = a_{11}x_1^o\Delta t + a_{21}x_2^o\Delta t + b_{11}u_1^o\Delta t + b_{12}u_2^o\Delta t + x_1^o - x_1^1 = 0$$

$$\frac{\partial K}{\partial \lambda_1^{N-1}} = a_{11}x_1^{N-1}\Delta t + a_{21}x_2^{N-1}\Delta t + b_{11}u_1^{N-1}\Delta t + b_{12}u_2^{N-1}\Delta t + x_1^{N-1} - x_1^N = 0 \qquad \text{....III-86}$$

$$\frac{\partial K}{\partial \lambda_2^o} = a_{21}x_1^o\Delta t + a_{22}x_2^o\Delta t + b_{22}u_2^o\Delta t + x_2^o - x_2^1 = 0$$

$$\frac{\partial K}{\partial \lambda_2^{N-1}} = a_{21}x_1^{N-1}\Delta t + a_{22}x_2^{N-1}\Delta t + b_{22}u_2^{N-1}\Delta t + x_2^{N-1} - x_2^{N-2} = 0$$

....III-87

Equations III-82 through III-87 were solved for three values of N (10, 20, 100) using the modified Newton-Raphson technique discussed earlier. The true optimal control was also available for this linearized example having been obtained by the Ricatti transformation method described by Koppel[5]. The program for this solution may be found in Appendix B.

Table III-5 compares the true optimal temperature and concentration trajectories with the approximate trajectories obtained for N = 10. Other approximations (N = 20, 100) are not shown because they agree with the true values to at least four significant figures. Figures III-9 and III-10 compare the true optimal control ($\hat{Q}$ and $\hat{w}$) with the approximate results for the three values of N.

Comments on Example V

It is important to note again in Table III-5 that a good approximation to the optimal control is obtained even at relatively large step sizes. Also note that the approximate solutions converge to the optimal as N increases.

Table III-5

Comparison of Temperature and Concentration Trajectories

Time, minutes	Temperature, T, ^{o}F		Concentration, C_A, lb mole/ft^3	
	Optimal	N=10	Optimal	N=10
0.0	20.00	20.00	0.5000	0.5000
0.1	21.88	21.88	0.4857	0.4858
0.2	23.68	23.74	0.4719	0.4716
0.4	27.22	27.39	0.4442	0.4432
0.6	30.70	30.99	0.4164	0.4146
0.8	34.15	34.56	0.3880	0.3856

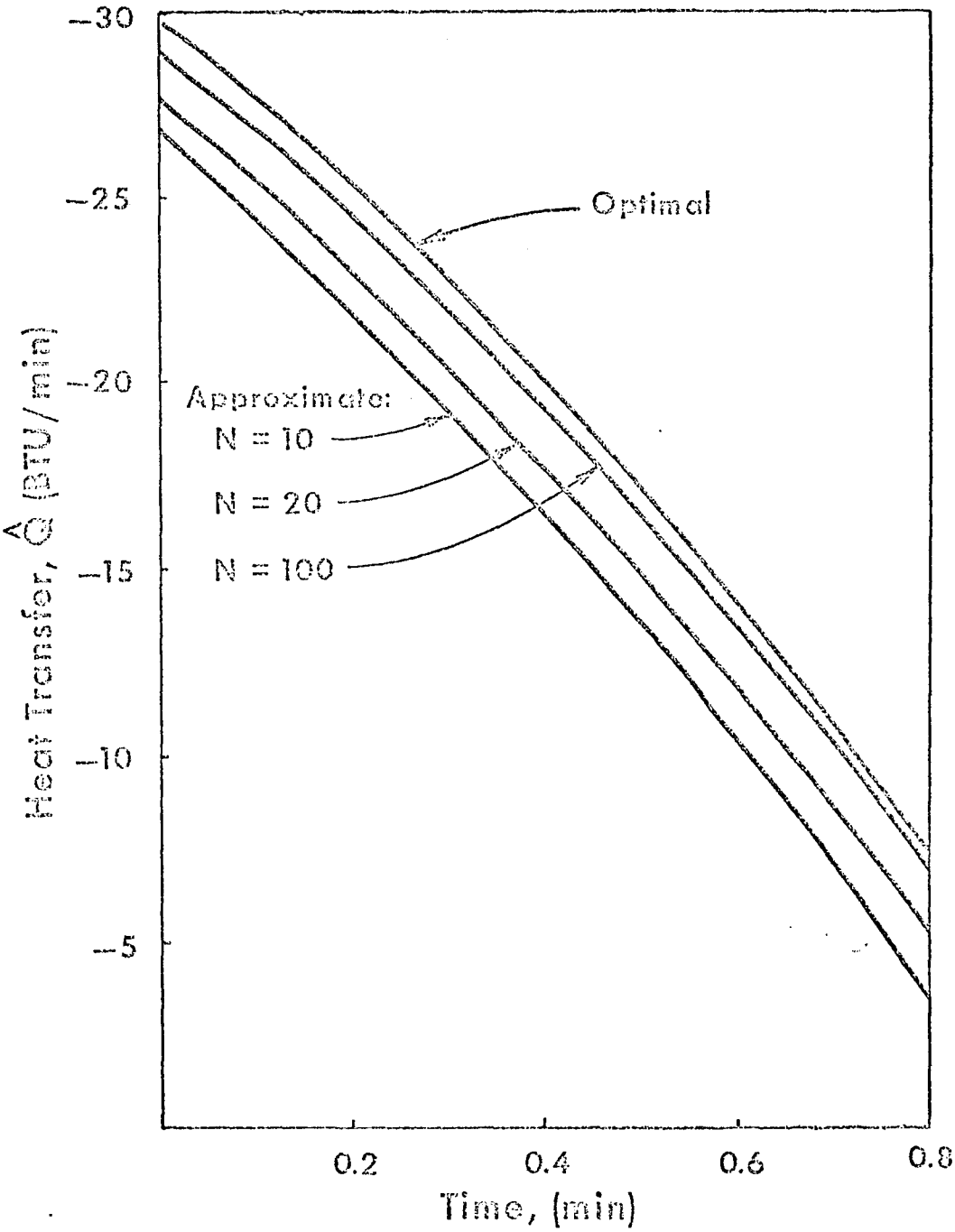

Figure III-9 Approximate and Optimal Control: Heat Transfer

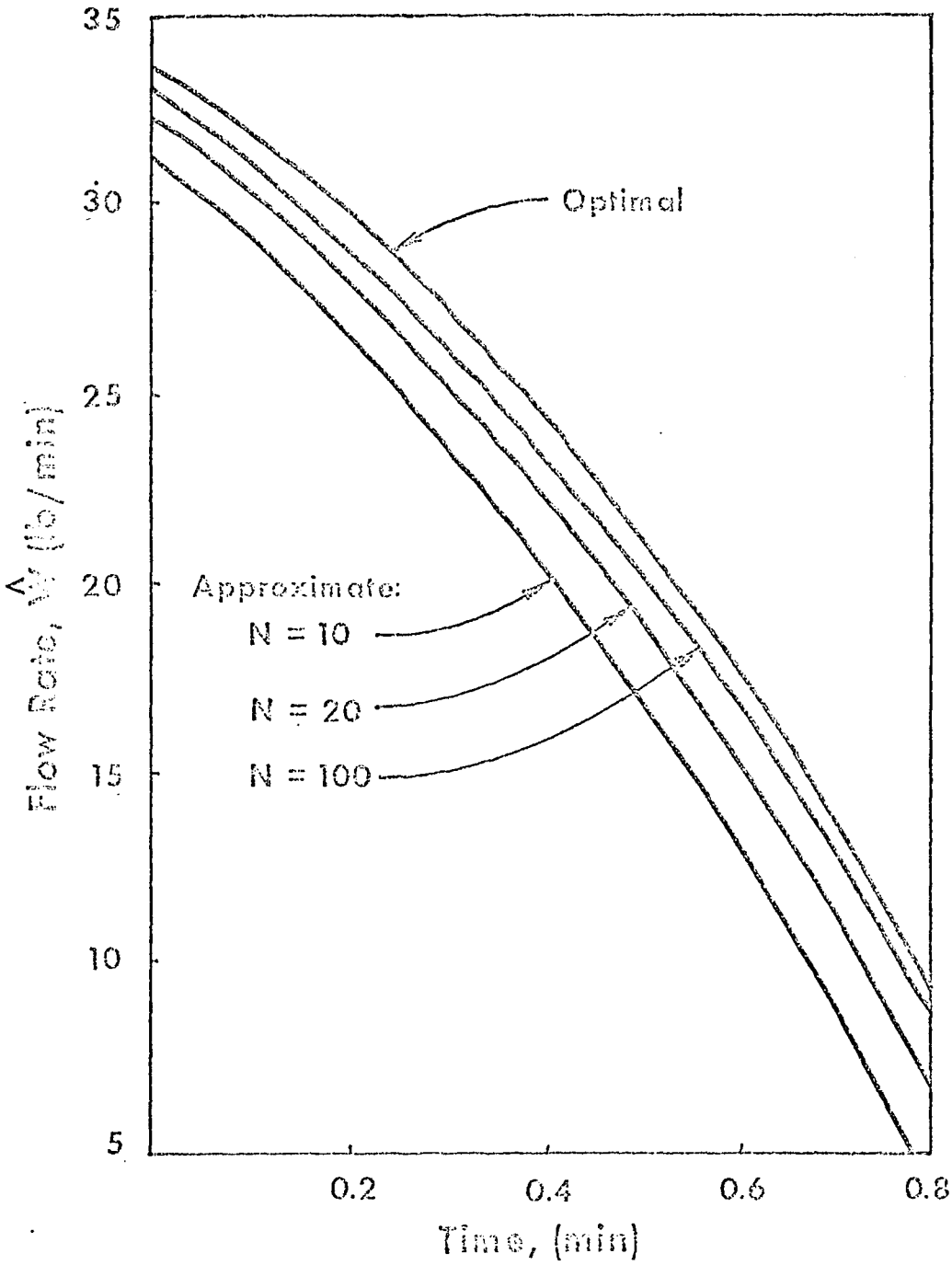

Figure III-10 Approximate and Optimal Control: Flow Rate

The greatest advantage of this finite difference method is its simplicity. The program to solve equations III-82 through III-87 via the Newton-Raphson method is given in Appendix B. This method converges very rapidly to the solution of the linear equations. For N=10, an initial guess of all unknowns equal to 1.0 and weighting factor equal to 0.9 resulted in sixty linear algebraic equations which were solved in about two to three seconds on an XDS Sigma 5 digital computer. For N=100, the same initial guess and weighting factor as in N=10 resulted in six hundred equations which were solved in approximately 40 seconds!

Since this example consisted of a linear equation and quadratic performance index, solution via the maximum principle could be obtained without solving a nonlinear two point boundary value (using the Riccati transformation). Even in this special class of problem (which is particularly easy to solve via the maximum principle), the programimg effort required is less using our direct approach. Compare programs for both methods in Appendix B.

It should be noted also that the direct method is not limited to any particular type of system or performance index.

Note in Table III-5 that the temperature is not "regulated" in the specified time (one minute). The reason for this is in order to bring the temperature toward the steady state value in this short amount of time (relative to the system time constants), would require an excessive control effort, thus, adding a greater penalty than the relative profit gained by regulation of temperature.

Optimal Control of Nonlinear Systems via the Direct Method

As has been mentioned previously, the direct finite difference method can handle linear or nonlinear systems. There is more incentive to use this method for the nonlinear system since we circumvent the solution of the sensitive nonlinear two point boundary value problem.

The choice of the solution method is not clear cut, however, since the direct method always yields nonlinear algebraic equations for the nonlinear system. The equations resulting from the examples considered in this study were, however, solved easily using Newton's method (previously discussed). There are many more sophisticated methods of solving nonlinear algebraic equations. References 11 and 12 are concerned with such methods.

Since nonlinearities may appear in many ways, it is not possible to characterize a typical or general class of nonlinear systems. Hence, application of the direct method to nonlinear systems will be illustrated by examples. The first is a "mildly" nonlinear system. The second is a highly nonlinear chemical reactor model describing an exothermic reversible reaction.

Example VI: Mildly Nonlinear System

Consider the system described by the following nonlinear differential equation:

$$\frac{dx}{dt} = -x(t)^2 + u(t) \qquad \text{....III-88}$$

where: $x(t=0) = 10$

The index of performance is given by:

$$J = \frac{1}{2}\int_o^{t_f=1.0}(x(t)^2 + u(t)^2)dt \qquad \text{....III-89}$$

Treating equation III-88 as a constraint yields:

$$K = \int_o^{t_f}\{x(t)^2+u(t)^2+\lambda(t)[-x(t)^2+u(t)^2-\frac{dx}{dt}]\}dt \qquad \text{....III-90}$$

The procedure is exactly the same as for the linear systems. First, approximate K numerically:

$$\begin{aligned} K \approx & \{(x^o)^2 + (u^o)^2 + \lambda^o[(-x^o)^2 + u^o - (\frac{x^1-x^o}{\Delta t})]\}\Delta t \\ & + \{(x^1)^2 + (u^1)^2 + \lambda^1[(-x^1)^2 + u^1 - (\frac{x^2-x^1}{\Delta t})]\}\Delta t \\ & + \vdots \\ & + \{(x^{N-1})^2+(u^{N-1})^2+\lambda^{N-1}[(-x^{N-1})^2+u^{N-1}-(\frac{x^N-x^{N-1}}{\Delta t})]\}\Delta t \end{aligned} \qquad \text{....III-91}$$

where: $\Delta t = 1/N$

The necessary conditions for an extremal are:

$$\begin{aligned} \frac{\partial K}{\partial x^1} &= -\lambda^o + 2x^1\Delta t - 2\lambda^1 x^1\Delta t + \lambda^1 = 0 \\ &\vdots \\ \frac{\partial K}{\partial x^{N-1}} &= -\lambda^{N-2} + 2x^{N-1}\Delta t - 2\lambda^{N-1}x^{N-1}\Delta t + \lambda^{N-1} = 0 \\ \frac{\partial K}{\partial x^N} &= -\lambda^{N-1} = 0 \end{aligned} \qquad \text{....III-92}$$

$$\frac{\partial K}{\partial u^o} = 2u^o\Delta t + \lambda^o\Delta t = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial u^{N-1}} = 2u^{N-1}\Delta t + \lambda^{N-1}\Delta t = 0 \qquad \text{....III-93}$$

$$\frac{\partial K}{\partial \lambda^o} = -(x^o)^2\Delta t + u^o\Delta t - (x^1 - x^o) = 0$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = -(x^{N-1})^2\Delta t + u^{N-1}\Delta t - (x^N - x^{N-1}) = 0 \qquad \text{....III-94}$$

Equations III-92 and III-94 are nonlinear while equations III-93 are linear. The equations corresponding to III-92 will be nonlinear for any system that has a nonlinear state term, x, since differentiation, with respect to a nonlinear term, will not be unity. Similarly, equations III-93 will be nonlinear if there is a nonlinear control term, u. Equations III-94 will always be nonlinear since the system differential equation is nonlinear.

Solution of the Necessary Conditions

The 3N equations III-92 through III-94 were solved for N equal to 20 and 100 by Newton's method. A weighting factor of 0.5 was chosen. Initial values for all the x's were 5. All the u's and λ's were assumed to be 1. For the case where N = 100, the resulting

three hundred algebraic equations were solved in about twelve seconds on the XDS Sigma 5 digital computer.

Solution of this problem was also obtained by a conventional solution of the two point boundary value problem resulting from application of the minimum principle. This problem is defined by:

$$\frac{dx}{dt} = -x^2 + u \qquad \text{....III-95}$$

$$\frac{d\lambda}{dt} = 2\lambda x - x \qquad \text{....III-96}$$

where: $x(t_o) = 10$

$\lambda(t_f) = 0$

$u = -\lambda$

A trial and error procedure was used to solve equations III-95 and III-96. Values of $x(t_f)$ were assumed, then equations III-95 and III-96 were integrated backward to t_o and the value of $x(t_o)$ was checked. The procedure was repeated until $x(t_o)$ was equal to 10. The results agree with those obtained by Sage[3] using quasilinearization.

Figure III-11 compares the state trajectory obtained by the finite difference method with the optimal. Figure III-12 compares the approximate control for N = 20 with the optimal. The control for N = 100 is not shown because it agrees with the optimal to at least two significant figures.

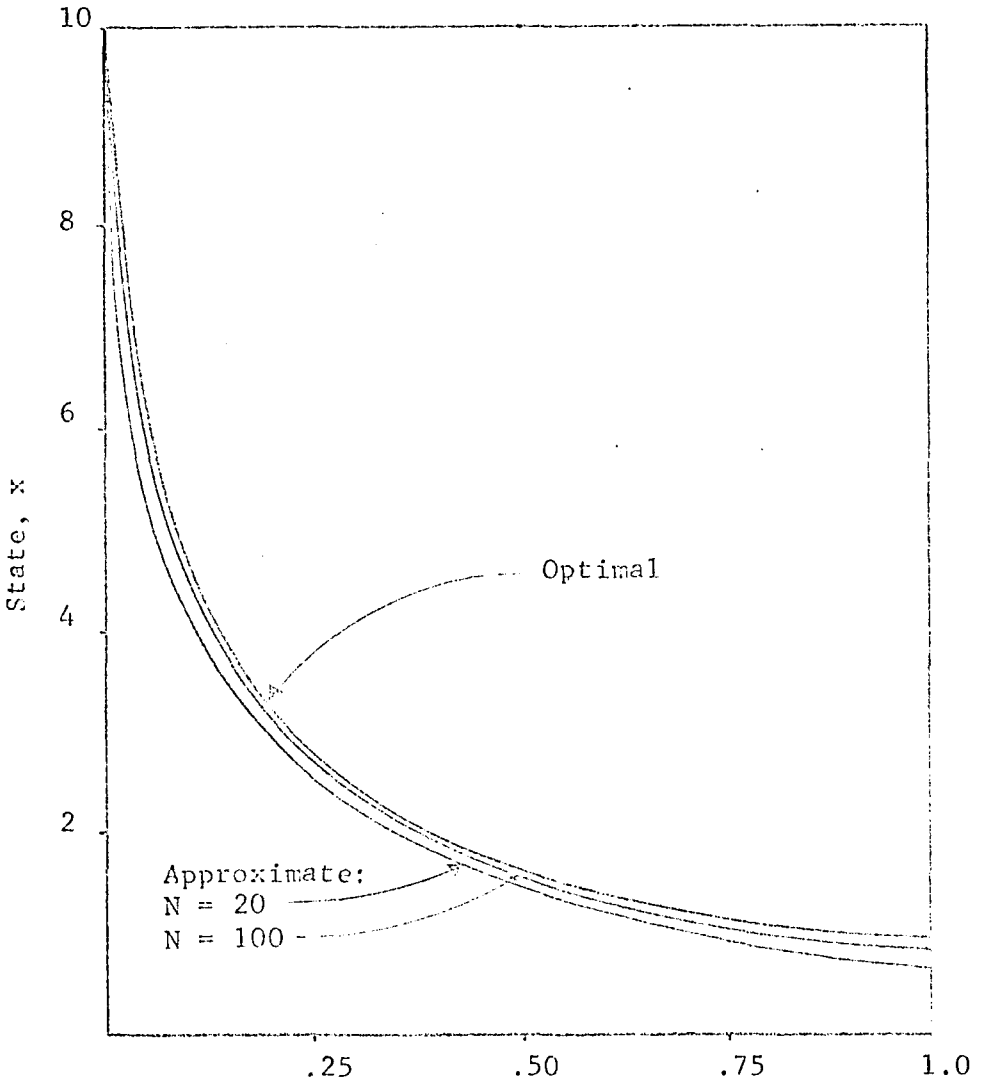

Figure III-11

Optimal and Approximate State Trajectories
for Nonlinear System

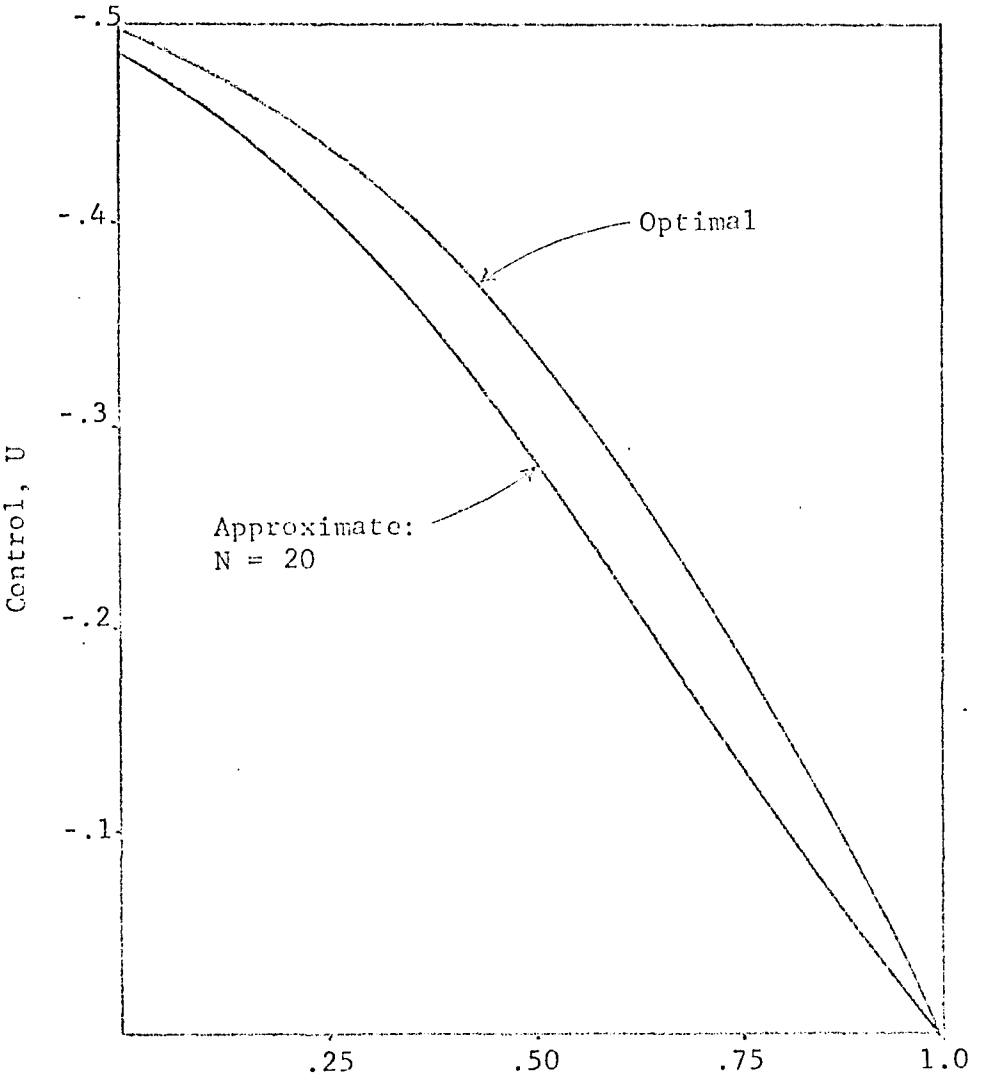

Figure III-12

Optimal and Approximate Control for Nonlinear System

Again, we observe that as the increment size is reduced the numerical procedure converges to the optimal. For N = 20, an acceptable approximation to the optimal control is obtained.

Optimal Temperature Program for a Reversible Reaction

We shall now consider calculation of the optimal temperature profile for the first order reversible exothermic reaction. This problem was treated in Chapter II by application of the maximum principle. For comparison purposes, we will assume the same kinetic parameters that were used in Chapter II. Consider the first order reversible reaction:

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} P$$

The reaction is assumed to be carried out in a batch reactor. We wish to determine the optimal temperature program for the reactor, i.e., the temperature vs time relation that will yield the most conversion in a given time.

Mathematically, the progress of the reaction may be described by the differential equation:

$$\frac{dx}{dt} = k_1(T)(1-x) - k_2(T)x \qquad \text{....III-97}$$

where

$k_1(T)$ = forward rate constant,

$k_2(T)$ = reverse rate constant,

x = fraction conversion of reactant A,

T = absolute temperature

t = time

The variation of rate constants with temperature is assumed to be given by the Arrhenius relation:

$$k_1(T) = k_{10} \exp(-E_1/RT)$$

$$k_2(T) = k_{20} \exp(-E_2/RT) \qquad \text{....III-98}$$

where

k_{10} = frequency factor for forward reaction,

k_{20} = frequency factor for reverse reaction,

E_1 = activation energy for forward reaction,

E_2 = activation energy for reverse reaction.

Substitution of equation III-98 into equation III-97 yields the nonlinear differential equation that describes this system. We wish to determine the control T(t) that will maximize the final conversion $x(t_f)$. Stating this in the nomenclature of our previous examples, the state variable is x, the control variable is T, and the performance index to be minimized is:

$$J = -x(t_f) \qquad \text{....III-99}$$

Proceeding as before, adjoin the system equation to the performance index to get a modified performance index K:

$$K = -x(t_f) + \int_o^{t_f} \lambda(t)[k_1(T)(1-x) - k_2(T)x - \frac{dx}{dt}]dt \quad \text{....III-100}$$

K is then approximated numerically and the necessary conditions for an extremal are obtained:

$$\frac{\partial K}{\partial x^1} = -\lambda^o + \lambda^1 - k_1^1\lambda^1\Delta t - k_2^1\lambda^1\Delta t = 0$$

$$\frac{\partial K}{\partial x^{N-1}} = -\lambda^{N-2} + \lambda^{N-1} - k_1^{N-1}\lambda^{N-1}\Delta t - k_2^{N-1}\lambda^{N-1}\Delta t = 0$$

$$\frac{\partial K}{\partial x^N} = -1 - \lambda^{N-1} = 0 \quad \text{....III-101}$$

$$\frac{\partial K}{\partial u^o} = k_1^o E_1(1-x^o) - k_2^o E_2 x^o = 0$$

$$\frac{\partial K}{\partial u^{N-1}} = k_1^{N-1} E_1(1-x^{N-1}) - k_2^{N-1} E_2 x^{N-1} = 0 \quad \text{....III-102}$$

$$\frac{\partial K}{\partial \lambda^o} = k_1^o(1-x^o)\Delta t + k_2^o x^o \Delta t - (x^1 - x^o) = 0$$

$$\frac{\partial K}{\partial \lambda^{N-1}} = k_1^{N-1}(1-x^{N-1})\Delta t + k_2^{N-1}x^{N-1}\Delta t - (x^N - x^{N-1}) = 0$$

....III-103

Solution of equations III-101 through III-103 was obtained by Newton's method. The following values of the parameters were used:

$$k_{10} = 69.5 \text{ sec}^{-1}$$
$$k_{20} = 5555 \text{ sec}^{-1}$$
$$E_1 = 10{,}000 \text{ Btu/lb mole}$$
$$E_2 = 20{,}000 \text{ Btu/lb mole}$$
$$t_f = 15 \text{ seconds}$$
$$x(t_o) = 0.1$$
$$N = 300$$

The approximate numerical solution compares very favorably with the analytical solution as shown in Table III-6. Values of optimal temperatures are compared at the same conversion. Also shown is the time necessary to get to this conversion.

Solution of the nonlinear algebraic equations III-101 was not obtained as easily as in other sample problems. This is caused by the highly nonlinear exponential term which causes steep temperature gradients. Some experimentation was necessary in choosing the weighting factor Z in the modified Newton-Raphson procedure. Convergence could not be obtained with Z = 1.0 or Z = 0.6 (with the chosen initial trial values of x, λ, and u) but with Z = 0.5 convergence was rapid. The initial trial values were as follows:

$$x^1 \ldots\ldots x^N = 0.5$$
$$\lambda^o \ldots\ldots \lambda^{N-1} = 2.0$$
$$T^1 \ldots\ldots T^{N-1} = 2000^\circ R$$

Table III-6

Comparison of Numerical and Analytical Solutions of Optimum Temperature Program Problem

Conversion	T, ^{o}R	T*, ^{o}R	Time, sec.	Time*, sec.
0.1	1740	1750	0.0	0.0
0.23	1295	1302	0.10	0.11
0.3	1184	1191	0.30	0.32
0.4	1065	1078	0.70	0.74
0.5	986	992	1.35	1.35
0.6	913	918	2.60	2.67
0.7	844	850	5.10	5.14
0.8	774	779	10.80	10.95

*denotes analytical solution.

The stability of the solution was also affected by the choice of $x(t_o)$. If the initial conversion is chosen as zero, the corresponding initial optimal temperature is infinite. This prevents numerical solution of the necessary equations. To circumvent this problem, a small initial conversion must be assumed.

Conclusion

In this chapter, the direct finite difference method was developed and applied to many linear and nonlinear optimal control problems. It was shown that the method can be applied in a straightforward manner to a wide variety of problems.

The results indicate that in most cases a good approximation to the optimal control can be obtained even with relatively large step sizes. In all cases considered, the approximation converged to the optimal as the step size was decreased.

This method results in an approximation to the optimal control function, $u^*(t)$. This optimal control function is a programmed or open loop control law since the control is a function only of time. Such control laws remain optimal only if the system follows the optimal trajectory. In the next two chapters, methods will be considered to obtain an approximation to the optimal feedback or closed loop control law, $u^*(x)$, for nonlinear systems.

Nomenclature

A - Constant in Arrhenius temperature equation

C_A - Concentration of A

$\bar{C}_A$ - Steady state concentration of A

$\hat{C}_A$ - Deviation from steady state concentration

C_P - Heat capacity

H - Hamiltonian function

J - Performance index

K - Adjoined performance index

L - General term in performance index

M - Number of increments from switching time to final time

N - Number of increments

Q - Heat transfer

$\bar{Q}$ - Steady state heat transfer

$\hat{Q}$ - Deviation from steady state heat transfer

T - Temperature

$\bar{T}$ - Steady state temperature

$\hat{T}$ - Deviation from steady state temperature

T_F - Feed temperature

V - Volume

w - Flow rate

$\bar{w}$ - Steady state flow rate

$\hat{w}$ - Deviation from steady state flow rate

Z - Weighting factor for Newton's method

a - Interval limits

$a_{n,m}$ - Element of A matrix

b - Interval limits

$b_{n,m}$ - Element of B matrix

R - Constant defined in Equation III-63

K_{10} - Frequency factor of forward reaction

K_{20} - Frequency factor of reverse reaction

p - Constant defined in Equation III-63

t - Time

t_o - Initial time

t_s - Switching time

t_f - Final time

x - State variable

u - Control variable

u_{max} - Maximum value of control variable

u_{min} - Minimum value of control variable

α - Constant defined by Equation III-32

β - Constant defined by Equation III-32

ΔH - Heat of reaction

Δt - Time increment

ρ - Density

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CHAPTER IV

APPROXIMATE OPTIMAL CLOSED LOOP CONTROL OF NONLINEAR SYSTEMS VIA PARAMETER SEARCH

Introduction

Optimal control theory has been given considerable attention in the literature of recent years. To date, however, little application has been made particularly in the area of process control. This is due to the limitation of the problems that can be solved. The typical optimal control problem is as follows:

Given the linear system defined by:

$$\dot{\underline{X}} = \underline{A}\,\underline{X} + \underline{B}\,\underline{u} \qquad \text{....IV-1}$$

where: $\underline{X}$ = n-dimensional state vector

$\underline{A}$ = n x n system matrix

$\underline{B}$ = n x r control matrix

$\underline{u}$ = r-dimensional control vector

$\dot{\underline{X}}$ = time derivative of $\underline{X}$

Find the control $\underline{u}(t)$ that will drive the system in such a way as to minimize a specified performance criterion or cost function. The optimal control problem is often classified according to the type of performance index specified.

Lapidus[1] lists the following measures of performance:

1) Terminal control: Drive the system as close as possible to a final state in a given time.

2) Minimum time: Drive the system to its final state in minimum time.

3) Minimum energy or fuel: Drive the system to its final state with a minimum control effort.

4) Regulator: Drive the system to an equilibrium state such that integral (or sum) of motion is minimized. Time not specified.

5) Pursuit: Drive the system to point y(t) in a minimum time.

The major drawback is that the control, $\underline{u}(t)$ is usually only a function of time or an open loop control such as that obtained in the previous chapter. Such a control is of little use in process control due to deviation of actual state behavior from the optimal. Such deviation is, in practice, always present due to modeling errors and unknown disturbances. A programmed control cannot compensate for a deviation from the optimal trajectory. For this reason, a feedback or closed loop control of the form $\underline{u}(x)$ is desirable. This type control tends to compensate for these errors since the control action is based on the actual value of the state. Optimal control theory can lead to an optimal feedback control only in certain specialized cases. For example:

1) If the system equations are linear as in equation IV-1 and the performance index is of the quadratic form. In this case, the

so-called Riccati transformation may be used to obtain a closed loop control algorithm. This subject is treated by Lapidus[1] and Athans[2].

2) If the dimensionality of the system is small ($n \leq 2$), dynamic programming is useful in obtaining closed loop control. For a greater number of state variables, computer storage requirements become excessive.

It becomes obvious that for the general multidimensional nonlinear system we must look to other approximate methods of obtaining an optimal or near optimal control algorithm. Approximate methods are available for removing the dimensionality problem associated with dynamic programming. Some of these considered by Lapidus are: polynominal approximation; dynamic programming with continuous independent variables; and, conformal grid updating.

Bryson and Ho[3] present a method, termed "pertubation feedback control", that consists of linearizing about a precalculated optimal trajectory and treating the deviations from that trajectory as a linear feedback problem.

The most common procedure is to linearize the system equations about some nominal operating point (i.e., steady state conditions) and apply linear optimal control theory to the linearized system. For highly nonlinear systems or systems in which a nominal operating range cannot be easily defined, these methods may be unsatisfactory.

It should be noted that in some cases, particularly in process control, there is much uncertainty in the development of a true mathematical model. Under such circumstances, there is no incentive to design a control

strategy based on a nonlinear model. There are cases, however, when the nonlinear model is well verified, such as temperature varying chemical reactors, and it may be worth the extra effort of using the more exact nonlinear model.

The purpose of the chapter is to present a simple straightforward procedure for obtaining a near optimal closed loop algorithm for a nonlinear system and compare it with linear design via optimal control theory.

The proposed method utilizes the "true" nonlinear system model. A multidimensional search technique is used to determine the optimal parameters in a proposed controller algorithm. Hence, the problem is reduced from a functional to a parameter optimization problem.

The "goodness" of the resulting control will be limited by the form or structure of the algorithm that is chosen. It will be shown that it is useful to determine the form of the control algorithm using the corresponding linear model and optimal control theory, where possible.

Computational Procedure

The procedure is as follows:

1) Propose a closed loop control algorithm such as:

$$\underline{u} = \underline{C}(t)\ \underline{x} \qquad \text{....IV-2}$$

where: $\underline{u}$ = 1 x n control vector

$\underline{C}(t)$ = n x n undetermined parameter matrix

$\underline{x}$ = n x 1 state vector

For linear time variation, the n x n elements of $\underline{C}(t)$ would be:

$$C_{nn}(t) = a_{nn} + b_{nn}\, t \qquad \text{....IV-3}$$

For this case, the 2 x n x n parameters a and b must be determined to specify $\underline{C}(t)$.

2) Assume value of parameters in $\underline{C}$ in equation IV-2. Drive the system by input of typical upset, such as initial conditions; set point change or disturbance. Evaluate the cost (performance index). Use search technique to improve the value of $\underline{C}$.

This procedure is illustrated diagrammatically in Figure IV-1 for initial conditions driving the system. If the actual system is upset in the same manner as the model is upset for the algorithm design, the resulting control should approach the optimal as the number of parameters is increased. It should be noted, however, that when unexpected disturbances enter the loop deviation from the optimal is increased. Hence, the way the model is driven for design purposes should depend on the "typical" expected operating conditions.

Multidimensional Example: Backmix Reactor

To illustrate the procedure discussed above, a nonlinear continuous stirred tank reactor was chosen. The system is illustrated in Figure IV-2 and is similar to that treated by Smith[4] and discussed in Chapter III.

The problem is to control the outlet temperature, T, and the

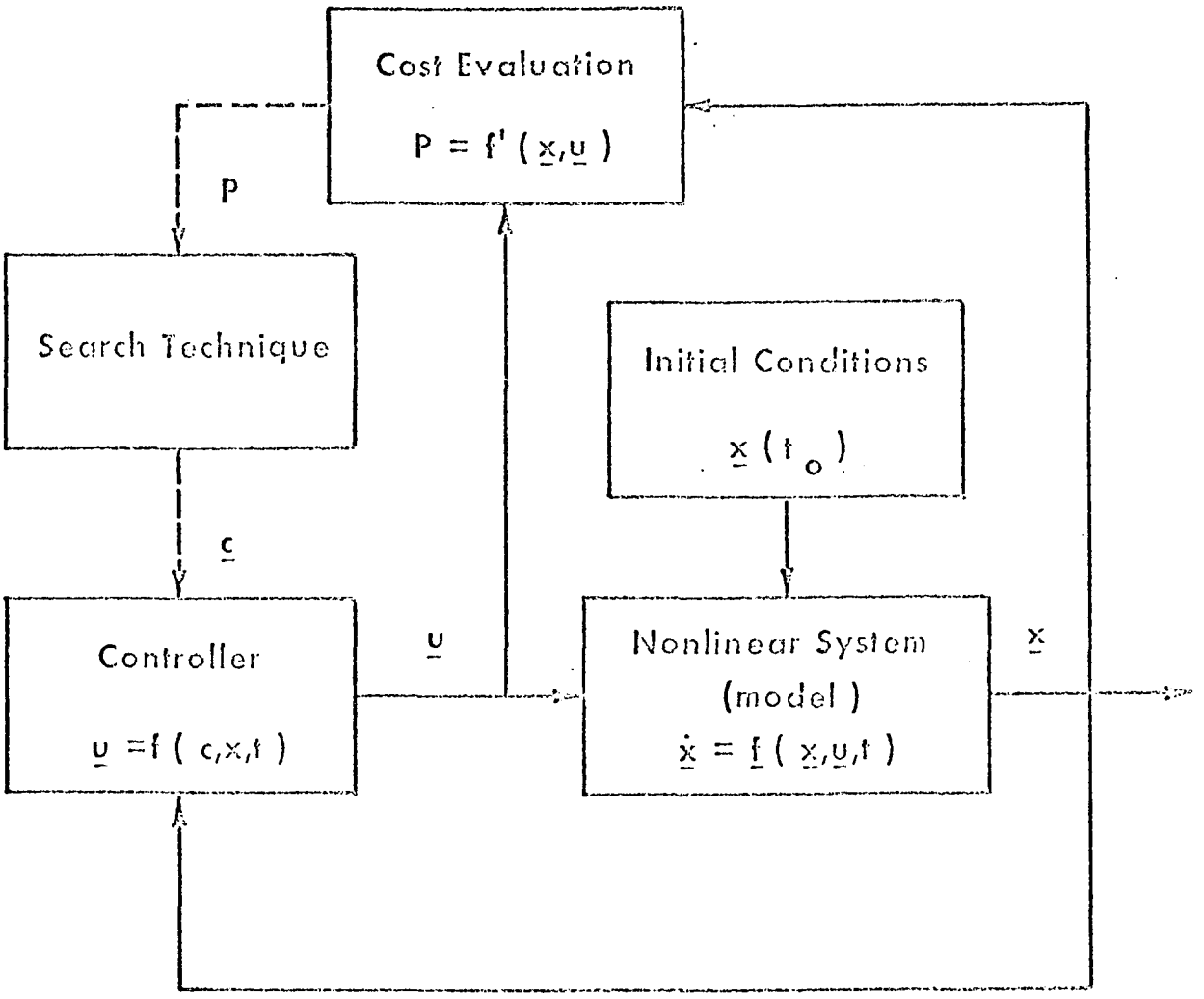

Figure IV-1

DETERMINATION OF CLOSED LOOP ALGORITHM VIA SEARCH TECHNIQUE

Note : Solid lines indicate continous information flow. Dotted lines indicate information flow after response generation.

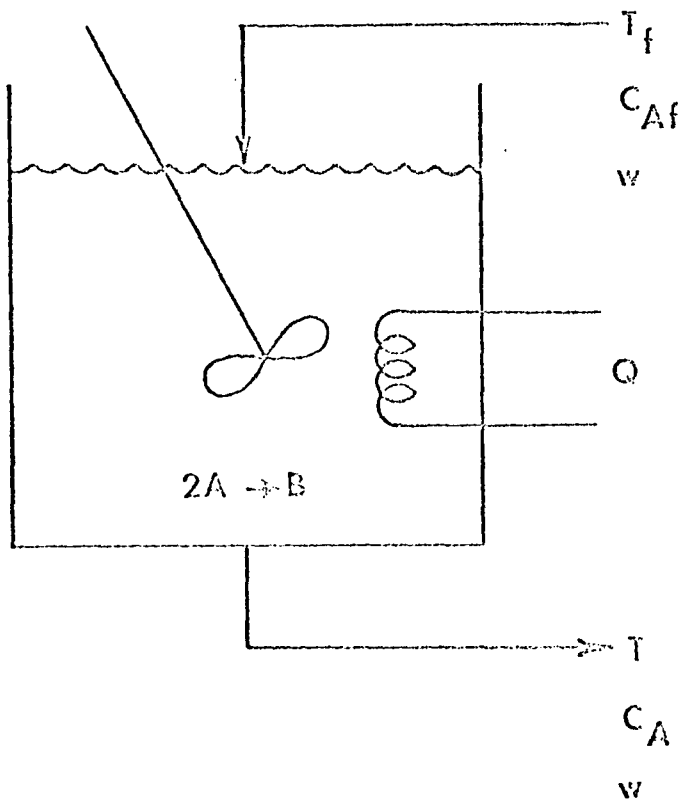

Figure IV- 2 Continuous Stirred-Tank Reactor

outlet concentration, C_A, at some desired set points, $\bar{T}$ and $\bar{C}_A$, in such a way as to minimize a specified cost function. The quadratic cost function is chosen so that we may perform linear analysis via Riccati's transformation for comparison purposes. This is of the form:

$$J = \frac{1}{2}\{\underline{x}(t_f),\ \underline{F}\ \underline{x}(t_f)\} + \frac{1}{2}\int_{t_o}^{t_f} [\{\underline{x}(t),\ \underline{Q}(t),\ \underline{X}(t)\} + \{\underline{u}(t),\ \underline{R}(t),\ \underline{u}(t)\}]dt \qquad \ldots\ldots \text{IV-4}$$

where:

$\underline{F}$ = a positive semidefinite matrix

$\underline{Q}(t)$ = a positive semidefinite matrix

$\underline{R}(t)$ = a positive semidefinite matrix

$\underline{x}$ = state vector

$\underline{u}$ = control vector

t_o = initial time

t_f = final time

The cost function described by equation IV-4 is very general; $\underline{F}$, $\underline{Q}$, and $\underline{R}$ are chosen so as to penalize the offset at t_f, deviation of state trajectory and deviation of control trajectory in the desired amount. These penalties are set by the system economics.

The manipulated variables are the feed rate, w, and the heat added or removed, Q. In practice not Q but the flow rate through a jacket or cooling coils would be manipulated. This is related to Q through an unsteady state energy balance. For this problem, however, it is simplier to assume Q is directly manipulated and that enough heat

transfer is available so that saturation does not occur. If R is chosen relatively large, this will assure that too great a control effort will not be used.

The system is driven by the initial conditions given for temperature and concentration. This is the state regulator problem of Athans and and Falb[2] and physically may be interpreted as a "start-up" problem. This type problem is considered for simplicity; however, the technique may be used for the more general set point or disturbance problem. The disturbance problem is treated by Johnson[5].

A second order irreversible reaction of the form:

$$2A \rightarrow B \qquad \text{....IV-5}$$

is assumed. The rate of reaction is expressed by:

$$\text{Rate} = \frac{dC_A}{dt} = kC_A^2 \qquad \text{....IV-6}$$

The rate constant, k, may be expressed as a function of temperature using the Arrhenius expression:

$$k = k_o \exp(-a/T) \qquad \text{....IV-7}$$

Substitution of equation IV-7 into equation IV-6 yields:

$$\text{Rate} = k_o \exp(-a/T) C_A^2 \qquad \text{....IV-8}$$

Note from equation IV-8 that the rate of reaction is nonlinear with

respect to temperature, T, and concentration in tank, C_A. The degree of nonlinearity with respect to T depends on the size of a, which is a function of the particular reaction.

Unsteady state material and energy balances on the reactor yield:

$$\frac{w}{v\rho}(C_{Af}-C_A) - kC_A^2 = \frac{dC_A}{dt} \qquad \text{....IV-9}$$

$$\frac{w}{v\rho}(T_f-T) + \frac{Q}{v\rho C_p} - \frac{\Delta H k C_A^2}{\rho C_p} = \frac{dT}{dt} \qquad \text{....IV-10}$$

Linear Analysis

The usual procedure for such a problem is to linearize the system equations IV-9 and IV-10 then solve by application of the minimum principle. This will be carried out for comparison purposes.

Linearization of equations IV-9 and IV-10 about steady state or set-point conditions yields:

$$\frac{d\hat{C}_A}{dt} = (-\frac{\bar{w}}{v\rho} - 2\bar{C}_A\bar{k})\hat{C}_A - (\frac{\bar{k}a\bar{C}_A^2}{\bar{T}^2})\hat{T} + (\frac{C_{Af}-\bar{C}_A}{v\rho})\hat{w} \qquad \text{....IV-11}$$

$$\frac{d\hat{T}}{dt} = (\frac{-2\ \Delta H\bar{k}\bar{C}_A}{\rho C_p})\hat{C}_A - (\frac{\bar{w}}{v\rho} + \frac{\Delta H\bar{k}\bar{C}_A^2 a}{\rho C_p \bar{T}^2})\hat{T} + \frac{\hat{Q}}{v\rho C_p} + (\frac{T_f-\bar{T}}{v\rho})\hat{w} \qquad \text{....IV-12}$$

$\hat{C}_A$ and $\hat{T}$, $\hat{Q}$, $\hat{w}$ are defined as variations about the steady state values, $\bar{C}_A$ and $\bar{T}$, $\bar{Q}$, $\bar{w}$. $\bar{w}$ and $\bar{k}$ are obtained from the steady state versions of equations IV-11 and IV-12. Equations IV-8 and IV-9 may be put into matrix notation as:

$$\frac{d}{dt}\begin{bmatrix}\hat{T}\\ \hat{C}_A\end{bmatrix} = \begin{bmatrix}\left(\frac{-\bar{w}}{v\rho} - \frac{a\Delta\bar{H}\bar{k}\bar{C}_A^2}{\rho C_p \bar{T}^2}\right) & \left(\frac{-2\Delta\bar{H}\bar{k}\bar{C}_A}{\rho C_p}\right)\\ \left(\frac{-a\bar{k}\bar{C}_A^2}{\bar{T}^2}\right) & \left(-\frac{\bar{w}}{v\rho} - 2\bar{k}\bar{C}_A\right)\end{bmatrix}\begin{bmatrix}\hat{T}\\ \hat{C}_A\end{bmatrix} + \begin{bmatrix}\frac{1}{v\rho C_p} & \frac{T_F-\bar{T}}{v\rho C_p}\\ 0 & \frac{C_{Af}-\bar{C}_A}{v\rho}\end{bmatrix}\begin{bmatrix}\hat{Q}\\ \hat{w}\end{bmatrix} \quad \ldots\ldots\text{IV-13}$$

Defining T and C_A as our state variables and Q and w as manipulated variables, we may write equation IV-13 as:

$$\dot{\underline{X}} = \underline{A}\,\underline{X} + \underline{B}\,\underline{u} \quad \ldots\ldots\text{IV-14}$$

For the linear system defined by equation IV-14 and the quadratic performance index defined by equation IV-4, optimal control theory tells that the optimal control is given by:

$$\underline{u}(t) = -\underline{R}^{-1}(t)\,\underline{B}^T(t)\,\underline{K}(t)\,\underline{x}(t) \quad \ldots\ldots\text{IV-15}$$

$\underline{K}(t)$ is the positive definite symmetric matrix that is the solution of the matrix Riccati equation:

$$\underline{K}(t) = -\underline{K}(t)\,\underline{A}(t) - \underline{A}^{T}(t)\,\underline{K}(t) + \underline{K}(t)\,\underline{B}(t)\,\underline{R}^{-1}(t)\,\underline{B}^{T}(t)\,\underline{K}(t) - \underline{Q}(t) \quad \ldots\ldots\text{IV-16}$$

The boundary condition for equation IV-16 is:

$$\underline{K}(t_f) = \underline{F} \quad \ldots\ldots\text{IV-17}$$

For t_f approaching infinity and constant coefficients in $\underline{A}$ and $\underline{B}$, equation IV-16 reduces to a set of algebraic equations:

$$0 = -\underline{K}\,\underline{A} - \underline{A}^{T}\,\underline{K} + \underline{K}\,\underline{B}\,\underline{R}^{-1}\,\underline{B}^{T}\,\underline{K} - \underline{Q} \quad \ldots\ldots\text{IV-18}$$

The solution of equation IV-18 yields $\underline{K}$ which may be substituted into equation IV-15 to yield the closed loop algorithm. For this example, let:

$$\underline{F} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad \ldots\ldots\text{IV-19}$$

$$\underline{R} = \begin{bmatrix} .01 & 0 \\ 0 & 1.0 \end{bmatrix} \quad \ldots\ldots\text{IV-20}$$

$$\underline{Q} = \begin{bmatrix} 1.0 & 10 \\ 10 & 400 \end{bmatrix} \quad \ldots\ldots\text{IV-21}$$

The following reactor parameters were chosen:

$$v = 13.38 \text{ ft}^3$$

$$\rho = 55 \text{ lb/ft}^3$$

$$C_p = 1.0 \text{ Btu/lb } ^\circ\text{F}$$

$$\Delta H = -12{,}000 \text{ Btu}$$

$$a = 14{,}000 \ ^\circ\text{R}$$

$$k_o = 8.33 \times 10^8 \text{ ft}^3\text{/lb mole min}$$

$$T_F = 100^\circ\text{F}$$

$$C_{AF} = 0.4 \text{ lb moles/ft}^3$$

$$\bar{T} = 200^\circ\text{F}$$

$$\bar{C} = 0.2 \text{ lb moles/ft}^3$$

Solution of the steady state version of equation IV-13 yields steady state flow rate, rate constant and heat duty as:

$$\bar{k} = 0.51 \text{ ft}^3\text{/lb mole min}$$

$$\bar{w} = 75.2 \text{ lb/min}$$

$$\bar{Q} = 4238 \text{ Btu/min}$$

Using the above parameters our system equation IV-13 or IV-14 becomes:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} .041 & 44.6 \\ -.001 & -.307 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} .001 & - & .136 \\ 0 & & .001 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \ldots\ldots \text{IV-22}$$

Solution of equation IV-18 yields:

$$\underline{K} = \begin{bmatrix} 7.11 & 760 \\ 760 & 102000 \end{bmatrix}$$

The optimal closed loop algorithm equation IV-15 becomes:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} -0.996 & -103 \\ 0.760 & 75.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \text{....IV-23}$$

Now we may apply our optimal controller, equation IV-23, for the linearized system, equation IV-22, to our original nonlinear system, equations IV-9 and IV-10. Hopefully, a "near optimal" control will result.

Controller Determination Via Search Technique

An approximate optimal control for the nonlinear system defined by equations IV-9 and IV-10 will be obtained as follows:

1) Propose a controller similar to that obtained by linearization. For example:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \text{....IV-24}$$

where $\underline{C}$ consists of undetermined parameters.

2) For a given typical set of initial conditions, generate the system response using the nonlinear system equations and trial or first guess values of the elements in $\underline{C}$. Evaluate the cost from equation IV-4.

3) Vary the parameters of $\underline{C}$ using a search technique to improve value of cost. Continue until no improvement may be found in the cost.

The procedure outlined above is very straightforward and is easily implemented on the digital computer. Core storage is small; however, run time is generally relatively long (5 to 10 min on the XDS Sigma 5) depending upon the method of integration of system equations, the number of parameters to be determined and closeness of initial parameter guess. The Fortran programs used in this study are found in Appendix C.

Comparison of Results: Search vs. Linearization

Various initial conditions on T and C were used to drive the system to the desired steady state (T = 200, C = 0.2). The feed temperature and concentration were adjusted to coincide with the intial conditions in the reactor so as to be realistic (simulate a "true" reactor start-up). The quadratic cost index defined by equations IV-4, IV-19, IV-20 and IV-21 was evaluated using the controller obtained via linearization followed by solution of the Riccati equation IV-18 and also using the "optimal" controller obtained by the Pattern Search[6]

technique. Comparison of the cost obtained for the two design techniques is shown in Table IV-1 for the various initial conditions. Note that in every case the search technique gives a "better" control or lower cost. This must always be true since for the true linear case a search technique should give the same parameters as the Riccati solution. This has been verified by Miller[7]. Note also that the relative advantage in going to the search procedure is a function of the starting point or how far we start from the point of linearization.

Figure IV-3 illustrates the % improvement (of search procedure) over linearization diagrammatically for the different intial states. It is interesting to note that the % improvement (or conversely the penalty obtained due to linear analysis) cannot be predicted simply from the distance the system state is driven from the point of linearization. This is obvious from considering the corresponding points in the left and right hand quadrant of Figure IV-3. Each corresponding point is the same "distance" from the origin (steady state); however, for the points in the right hand quadrant there is greater incentive to depart from linear analysis and optimal control theory. This is a good illustration of the dependence of response characteristics of nonlinear systems on initial conditions. Often linearization of nonlinear systems (for analysis and design purposes) is justified by the fact that the control system will usually operate "near" its desired steady state value. Figure IV-3 illustrates that this justification may be risky in certain cases.

Table IV-1

Quadratic Cost Comparison*

Initial Conditions		Cost		% Advantage in Search
T	C	Linearization	Search	
100	0.3	10,746	9,735	9.5
150	0.3	2,083	2,030	2.5
250	0.3	4,409	4,112	6.7
300	0.3	15,921	13,822	13
100	0.4	16,401	13,109	20
150	0.4	1,812	1,741	3.9
250	0.4	19,224	13,679	28
300	0.4	50,700	35,622	30

*System driven to: T = 200
C = 0.2

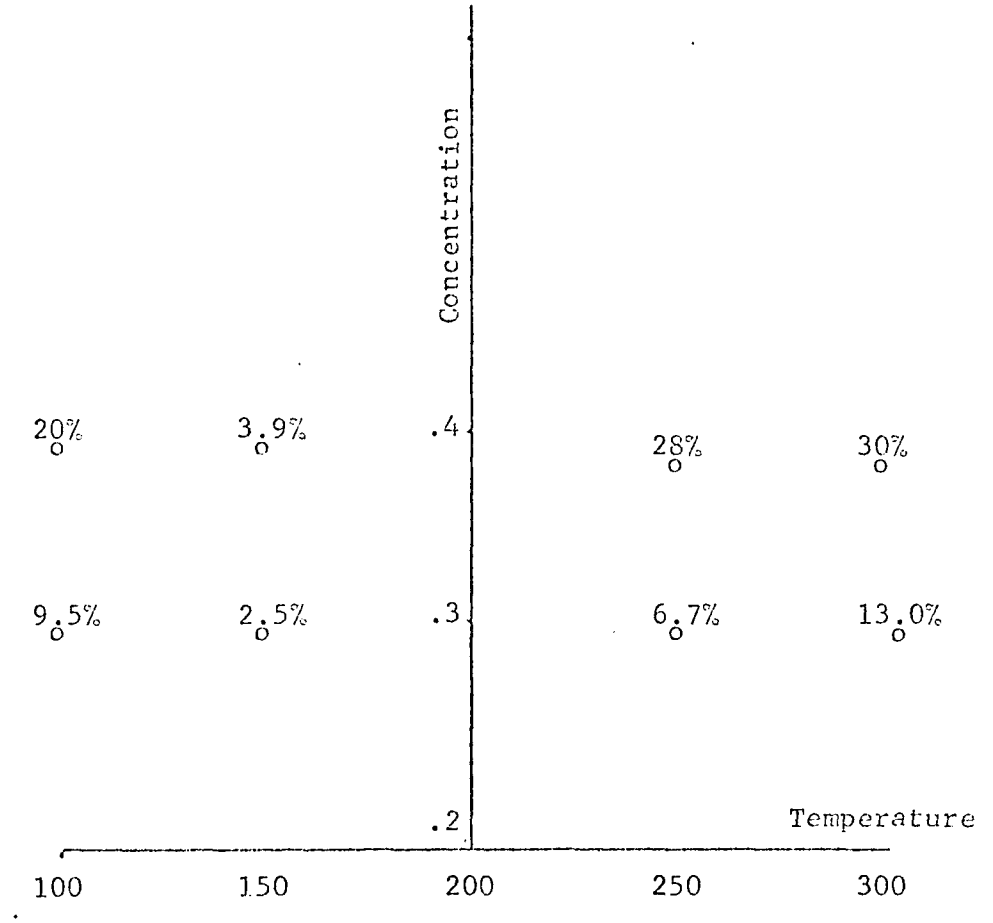

Figure IV-3

Percent Advantage of Search Technique over Linearization

For our particular case, a closer look at the nonlinear and corresponding linearized equations will illustrate this point. Consider the homogeneous version of equations IV-9 through IV-12:

$$\frac{dC_A}{dt} = \frac{-k_o}{e^{a/T}} C_A^2 - \frac{w}{v\rho} C_A \qquad \text{....IV-25}$$

$$\frac{dT}{dt} = \frac{-\Delta H}{\rho C_p} \frac{k_o C_A^2}{e^{a/T}} - \frac{w}{v\rho} T \qquad \text{....IV-26}$$

$$\frac{d\hat{C}_A}{dt} = \left(\frac{\bar{w}}{v\rho} - 2\bar{C}_A\bar{k}\right) \hat{C}_A - \left(\frac{\bar{k}a\bar{C}_A^2}{\bar{T}^2}\right) \hat{T} \qquad \text{....IV-27}$$

$$\frac{d\hat{T}}{dt} = \left(\frac{2\Delta H\bar{k}\bar{C}_A}{\rho C_p}\right)\hat{C}_A\left[-\frac{\bar{w}}{v\rho} + \left(\frac{\Delta H\bar{k}\bar{C}_A^2 a}{\bar{T}^2}\right)\right]\hat{T} \qquad \text{....IV-28}$$

Note that in equations IV-25 and IV-26, $\frac{-k_o}{e^{a/T}}$ and $\frac{-\Delta H}{\rho C_p}\ \frac{1}{e^{a/T}}$ may be considered as variable coefficients of the nonlinear term C_A^2. At the larger average values of T, this coefficient is large; hence, the C_A^2 term is amplified and the effect of departure from linearity becomes more pronounced. This explains the greater penalty for linearization in the right quadrant of Figure IV-3.

Optimality of Algorithm

It should be re-emphasized that the results of such a parameter search yield an approximate or near optimal control. For the "true" linear system we can be assured that the theory will yield the best or optimal control. Very few systems (particularly those encountered in

process control) are truly linear. Most are actually distributed, nonlinear and not completely deterministic.

Obviously the results of a parameter search for the nonlinear system are going to depend upon the way the system is forced (initial conditions in this example). If the initial conditions are known precisely, optimal control theory will lead directly to the optimal control $\underline{u}(t)$ and the state trajectory $x(t)$, provided we can solve the formidable two point boundary value problem. Hence, if no upsets occur we essentially have a closed loop optimal control.

In general, the initial conditions or forcing functions are not known before hand. However, an estimate based on "engineering judgement" is usually available. Results of this study indicate that a parameter search based on an estimated set of initial conditions can give better results than the linearization technique. Table IV-2 illustrates this point. Controllers designed via parameter search at three different initial points were applied to the other seven initial points. It is noted that in most cases the performance is better than with the optimal controller obtained from linearization. Note that in every case where the initial conditions are in the same quadrant of Figure IV-2 as the basis for the search better results are obtained.

This indicates that the technique is still of value even if the exact forcing function is not known before hand, which is of course the general case. For example, if it is desired to design a controller to start up a chemical reactor (optimally) one might define a typical start up or initial condition as a basis for the search. This procedure should

Table IV-2

Cost Comparison for Controller Design Based on Different Initial Conditions

Initial Conditions		Design Basis (Initial Conditions)			Linearization
T	C	T = 150 C = 0.4	T = 250 C = 0.3	T = 300 C = 0.3	
100	0.3	9,763	10,621	13,246	10,746
150	0.3	2,030	3,275	2,215	2,083
250	0.3	4,447	4,112	4,178	4,409
300	0.3	15,232	13,875	13,822	15,621
100	0.4	13,266	15,333	23,434	16,401
150	0.4	1,779	2,122	5,479	1,812
250	0.4	15,708	13,789	14,464	19,224
300	0.4	44,073	36,601	36,180	50,700

give better results than linearization (about the same typical initial conditions) particularly if start up covers a large region of state space and if the reactor is highly nonlinear.

Other Forms of Control Algorithm

It should be mentioned that when designing a control algorithm via parameter search, we are in no way limited to a particular form of control equation. Controllers other than that in equation IV-22 were considered. Two of these are:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ C_5 & C_6 & C_7 & C_8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_1|x_1| \\ x_2 \\ x_2|x_2| \end{bmatrix} \quad \ldots\ldots\text{IV-29}$$

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ C_5 & C_6 & C_7 & C_8 \end{bmatrix} \begin{bmatrix} x_1 \\ \dot{x}_1 \\ x_2 \\ \dot{x}_2 \end{bmatrix} \quad \ldots\ldots\text{IV-30}$$

The rather surprising results are that no controller gave better performance than equation IV-22, that form predicted for the linearized

version of our nonlinear system. Although this is not always the case, it gives us a good starting point and we can be assured of coming up with at least as close to the true optimal as with linear optimal control theory.

Time Varying Closed Loop Control

Often the optimal closed loop control algorithm for linear systems is time varying of the form:

$$\underline{u}(x,t) = \underline{C}(t)\ \underline{x}(t) \qquad \text{....IV-31}$$

It is logical to consider such algorithms for optimal control for nonlinear systems. This typical algorithm provides no problem for our parameter search procedure except that computation time is increased as the number of parameters are increased. The search procedure is used in the same manner as in the previous time invariant problems. The only modification is that C is an unknown function of time. A polynominal approximation for C is made of the form:

$$C(t) = a_1 + b_1 t + c_1 t^2 + \ldots\ldots \qquad \text{....IV-32}$$

where: $t_o \leq t \leq t_f$

The unknown constants are now determined by search technique. This procedure will be illustrated by a simple example.

Consider the nonlinear system defined by:

$$\frac{dx}{dt} = -\frac{1}{2}x^2(t) + u(t) \qquad \text{....IV-33}$$

where: $x(t)$ = state variable

$u(t)$ = control variable

The problem is to find a closed loop control algorithm $u = f(x,t)$ that will minimize the quadratic performance index:

$$J = 200 \int_{t_o}^{t_f} [x^2(t) + \rho u^2(t)]dt \qquad \text{....IV-34}$$

Again for comparison we will linearize equation IV-33 about a given steady state point and solve using the Riccati equation. Linearizing equation equation IV-34 about the point $x = 1$, yields:

$$\frac{d\hat{x}}{dt} = -\hat{x}(t) + \hat{u}(t) \qquad \text{....IV-35}$$

where $\hat{x}$ denotes variation from the steady state point.

The Riccati equation reduces to the first order differential equation:

$$\frac{dK(t)}{dt} - 2K(t) - \frac{1}{2\rho}K(t)^2 + 2 = 0 \qquad \text{....IV-36}$$

The solution of equation IV-36 is:

$$K(t) = \frac{2}{1+\alpha \coth [\alpha(t_f - t)]} \qquad \text{....IV-37}$$

From equation IV-15, u(t) becomes:

$$u(t) = -\frac{1}{2\rho}\left\{\frac{2}{1+\alpha \coth\left[\alpha(t_f - t)\right]}\right\}x(t) \qquad \text{....IV-38}$$

where: $\alpha = \sqrt{1 + \rho^{-1}}$

Equation IV-38 is our optimal closed loop time varying algorithm for the linear system defined by equation IV-35.

Returning attention to our original nonlinear system equation IV-33, we will propose a series of closed loop algorithms and use search techniques (pattern and golden section) to determine the parameters in each. Cost evaluation will also be made applying the optimal controller for the linearized system, equation IV-38, to the nonlinear system. System parameters are chosen as:

$$\rho = 0.2$$

$$t_f = 2.0$$

$$\bar{x} = 1.0$$

$$x(t_o) = 2,\ 3,\ 4,\ 5$$

The proposed control algorithms are:

$$u = a_1\, x(t) \qquad \text{....IV-39}$$

$$u = [a_1 + b_1 t]x(t) \qquad \text{....IV-40}$$

$$u = [a_1 + b_1 t + c_1 t^2 + d_1 t^3] \qquad \text{....IV-41}$$

Determination of the parameters for initial conditions, $x(t_o) = 2$, yields the following:

$$u(t) = -0.921\, x(t) \qquad \text{....IV-42}$$

$$u(t) = [-.885 - .16t]x(t) \qquad \text{....IV-43}$$

$$u(t) = [-1.03 + 1.56t - 3.47t^2 + 1.42t^3]x(t) \qquad \text{....IV-44}$$

The constant in equation IV-42 was determined using a golden section search routine and the constants in equations IV-43 and IV-44 were determined using pattern search. Table IV-3 illustrates the resulting costs using the various control algorithms at different initial conditions.

It is interesting to note in Table IV-3 that even a linear time variation gives a much better control (lower cost) than does the constant gain. Also there is very little incentive in this problem to go to nonlinear time variations. These observations are significant in that we can add a linear time variation in our gains at the cost of only one additional parameter to be obtained via search technique for each gain. It is also observed as in the previous example, that the farther we get from our point of linearization, the poorer the resulting control from optimal control theory. Notice again that the power of linear optimal control theory is still used in that the theory tells us the optimal control for the corresponding linearized system is proportional and time varying. This provides a starting point for the parameter

Table IV-3

Cost Comparison for Various Control Algorithms

Initial Conditions	u1(t)*	u2(t)*	u3(t)*	u4(t)*
2	80.5	156.9	77.38	77.14
3	167	324.8	159.58	159.58
4	275	532.2	260.6	260.5
5	399	768.0	374.4	374.1

---

*$u1(t) = \{\frac{1}{\rho + \alpha\rho \coth [\alpha(t_f - t]}\}x(t)$;

$u2(t) = a_1 x(t)$;

$u3(t) = [a_1 + b_1 t]x(t)$;

$u4(t) = [a_1 + b_1 t + c_1 t^2 + d_1 t^3]x(t)$.

search.

Conclusions

The following conclusions may be drawn from the preceding examples:

1) If computer time is available, a parameter search to determine an approximate control algorithm for a nonlinear system should give better results than corresponding linear techniques (which are only available in certain restricted cases).

2) The degree of imporvement over linear optimal control theory is a function of the degree of nonlinearity of the system, the distance the system must operate away from the point of linearization, and the particular region in state space being considered. The third of these cannot, in general, be estimated a priori.

3) Linear optimal control theory (when possible) is useful to establish a form of the proposed algorithm to be determined by search.

4) Using a parameter search to determine a near optimal closed loop control is not restricted by type of performance index or difficult solutions to two point boundary value problems. The only limitation is computer time.

5) Time varying controllers present no problems except in the increased dimensionality of the search. A linear time variation may shown considerable improvement over a time invariant control with minimum increase in parameters to be determined (one per gain).

The method developed in this chapter is admittedly rather crude in that classical optimal control theory is not involved. This is, however, the major advantage of the technique. There are no complicated differential equations to solve (other than the initial value system model) and the resulting algorithms can easily be implemented on the digital computer.

In the following chapter, a more sophisticated and theoretical procedure, based on the maximum principle, will be developed.

Nomenclature

$\underline{A}$ - System matrix defined by equation IV-1

$\underline{B}$ - Control matrix defined by equation IV-1

B - Product of reaction in equation IV-5

$\underline{C}$ - Undetermined parameter matrix

C_A - Concentration at reactant A

C_{Af} - Feed concentration

$\bar{C}_A$ - Steady state concentration

$\hat{C}_A$ - Deviation from steady state concentration

C_p - Heat capacity

$\underline{F}$ - Matrix defined by quadratic performance index, equation IV-4

$\underline{Q}$ - Matrix defined by quadratic performance index, equation IV-4

Q - Heat transfer

$\bar{Q}$ - Steady state heat transfer

$\hat{Q}$ - Deviation from steady state heat transfer

$\underline{R}$ - Matrix defined by quadratic performance index, equation IV-4

T - Absolute temperature

T_F - Feed temperature

$\bar{T}$ - Steady state temperature

$\hat{T}$ - Deviation from steady state temperature

a - Constant defined in equation IV-7

a_{nm} - Undetermined parameter for time varying control

b_{nm} - Undetermined parameter for time varying control

b - Rate constant defined by equation IV-7

$\bar{b}$ - Steady state rate control

b_o - Constant defined by equation IV-7

t - Time

t_o - Initial time

t_f - Final time

$\underline{u}$ - Control vector

v - Volume

w - Flow rate

$\bar{w}$ - Steady state flow rate

$\hat{w}$ - Deviation from steady state flow rate

x - State variable

$\bar{x}$ - Steady state value of state variable

α - Constant defined by equation IV-38

ΔH - Heat of reaction

ρ - Density

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CHAPTER V

A HYBRID CONTROLLER FOR APPROXIMATE OPTIMAL FEEDBACK CONTROL OF NONLINEAR SYSTEMS

Introduction

In this chapter, design of an approximate optimal feedback control strategy for nonlinear systems will again be considered. A very different and more theoretical approach will be used. The technique, although more complicated than that considered in the Chapter IV, has the advantage that it can correct for large unexpected disturbances.

The procedure consists of precalculation of an open loop optimal control strategy. This control is applied to the nonlinear system. The system is sampled at regular intervals. If the sampled value agrees with the precalculated optimal trajectory, no correction is made. If there is a deviation due to a disturbance, a new optimal control strategy is calculated from this point and applied until the next sampling point.

The problem is that the calculation of the new optimal control must be done in real-time so it can be applied "immediately" to the system. Unfortunately, solving for the new optimal control usually involves a time consuming trial and error solution of a nonlinear boundary value problem. This problem is usually of the form:

$$\frac{dx}{dt} = f(x, \lambda, t) \quad ; \quad x(t_o) = \text{specified}$$

$$\frac{d\lambda}{dt} = g(x, \lambda, t) \quad ; \quad \lambda(t_f) = \text{specified}$$

where: f and g are nonlinear functions

x is the state variable

λ is the adjoin or costate variable that is related to the optimal control

The problem of "on line" solution of such a trial and error problem is overcome by use of the "hybrid controller".

The procedure is to repeatedly solve the open loop optimal control problem "off line" at various points along the state trajectory. For example, if the optimal precalculated open loop state trajectory looks like that shown in Figure V-1, we might resolve the optimal control problem at points surrounding this trajectory corresponding to the o's.

Theoretically, we could store the resulting optimal control, $u^*(t)$, for each calculation point. Next, by sampling the system at these points along the trajectory, we could detect the effect (on the state) of any disturbance that may have entered the loop. We could then "look up" in the digital computer the optimal control corresponding to the actual value of the state variable. Such a procedure is highly impractial. Computer storage requirements would become excessive.

For each calculation point, it would be necessary to store a corresponding control vector; that is, an array of controls corresponding to u(t). For systems higher than first order, this would be practically

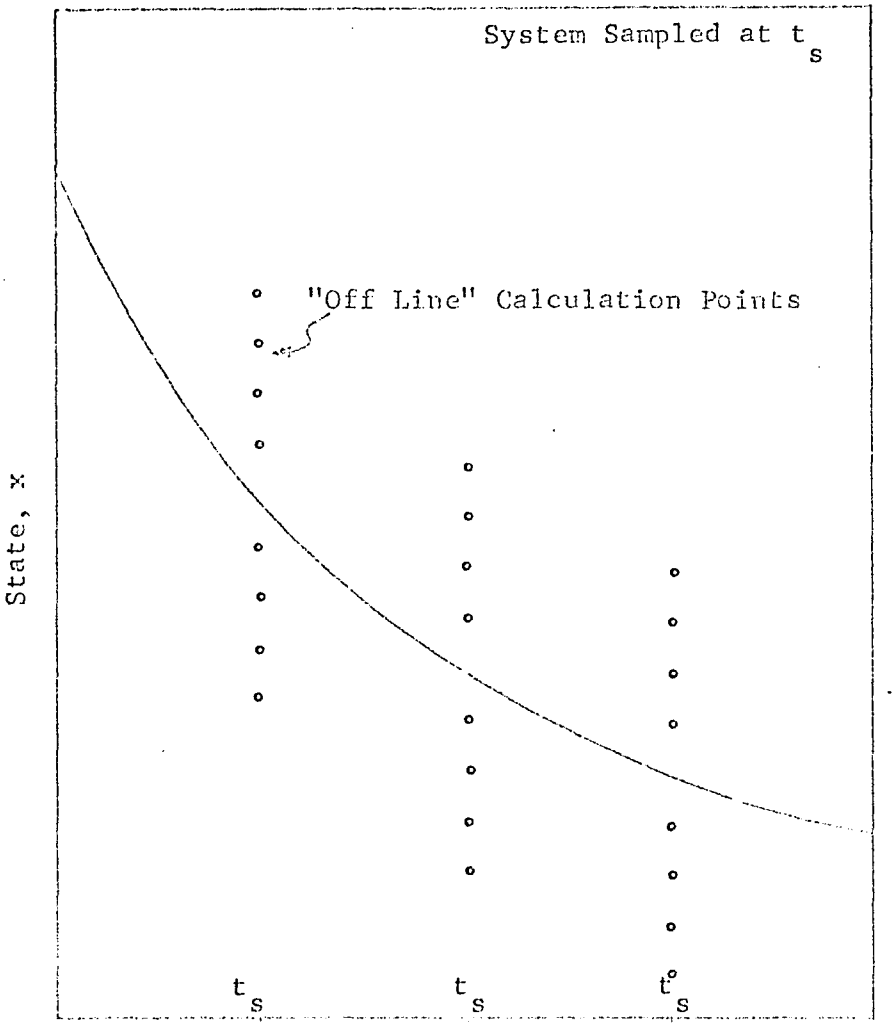


Figure V-1

Typical Open Loop Optimal
State Trajectory

impossible. Another problem would involve interpolation between two control vectors. Since the sampled values of the state, X, are not likely to fall exactly on a calculation point,it would usually be necessary to interpolate. Such interpolation is not straightforward since it would involve interpolation for every point in the array u(t).

To overcome these problems, we store only the value of the missing boundary condition in the digital computer memory corresponding to each calculation point. With this boundary condition available, solution of the optimal control problem is no longer a trial and error boundary value problem but an initial value problem that can be solved very rapidly on the analog computer. This allows us to solve the optimal control problem in real-time and apply this control to our system until the next sampling point.

The controller, therefore, operates as follows:

1) The precalculated optimal control is applied to the system initially.

2) The system is sampled at regular intervals. From the digital computer memory,the missing boundary condition is obtained corresponding to the value of the state. Either a table look-up and corresponding interpolation routine or a polynomial expression is used.

3) These boundary conditions are transferred to the analog where a rapid integration is made. Results of this integration are sampled and stored as an array in the digital computer memory. Note that it is only necessary to store values of the control until the next sampling point

since at this point the procedure is repeated.

4) These stored values of the new optimal control are used to drive the system until the next sampling point.

Figure V-2 illustrates this procedure diagrammatically.

Application to a First Order Nonlinear System

Implementation of this hybrid controller will be illustrated by an example. Consider the first order nonlinear system defined by the following differential equation:

$$\frac{dx(t)}{dt} = -x^2(t) + u(t) \qquad \ldots.V\text{-}1$$

where: $x(0) = 10$

$t_f = 1.0$

The system is to be driven in such a way as to minimize the quadratic performance index:

$$J = \frac{1}{2}\int_0^{1.0} [x^2(t) + u^2(t)]dt \qquad \ldots.V\text{-}2$$

The open loop control strategy, $u^*(t)$, is obtained from application of the maximum principle. The Hamiltonian may be written as:

$$\mathcal{H} = \lambda(-x^2 + u) + \frac{1}{2}(x^2 + u^2) \qquad \ldots.V\text{-}3$$

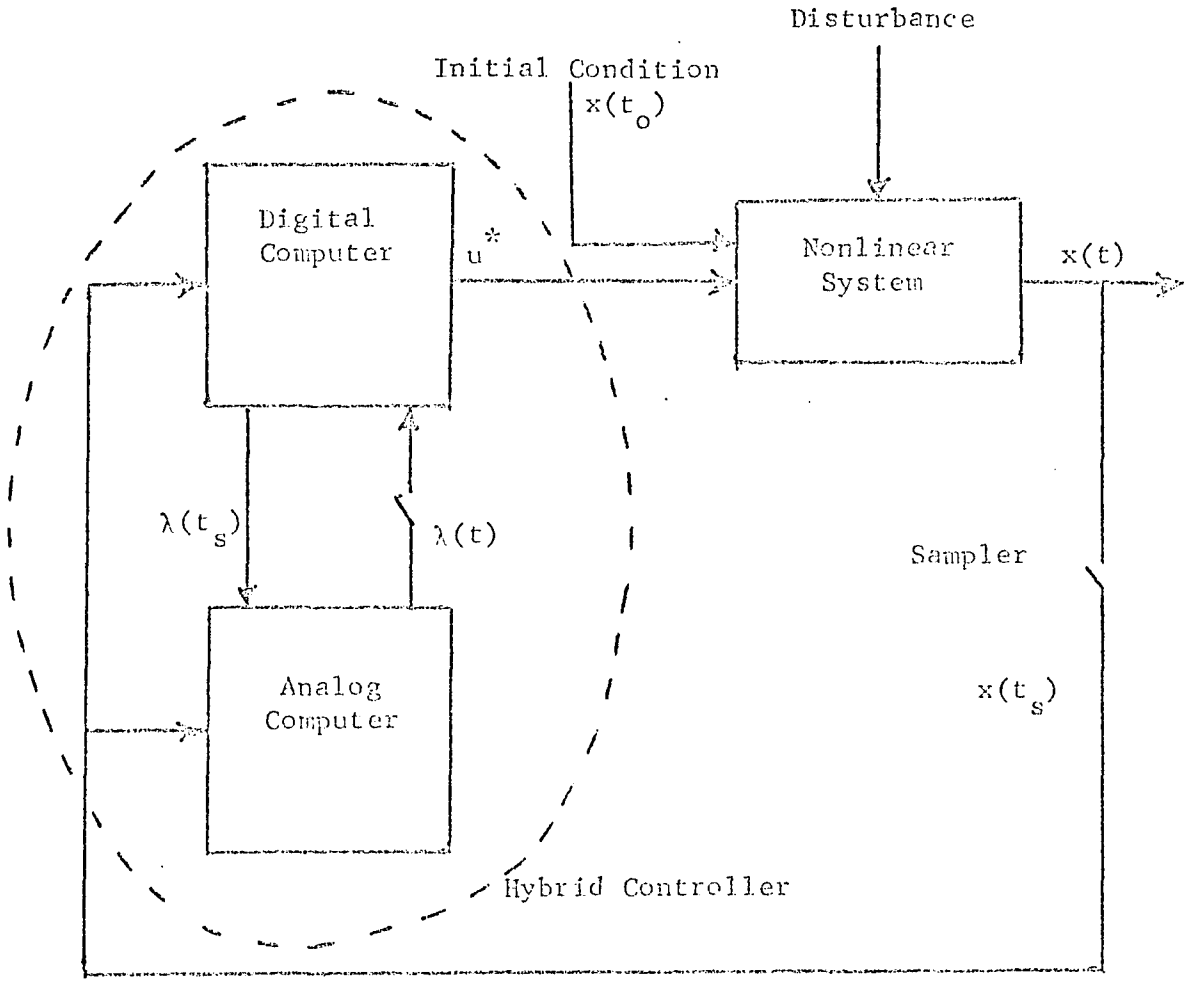


Figure V-2

Hybrid Controller For System Driven by Initial Conditions

The necessary conditions that define the optimal control are:

$$\frac{dx}{dt} = -x^2 + u \quad ; \quad x(0) = 10 \qquad \text{....V-4}$$

$$\frac{d\lambda}{dt} = 2\lambda x - x \quad ; \quad \lambda(t_f) = 0 \qquad \text{....V-5}$$

$$\frac{\partial H}{\partial u} = 0 = \lambda + u^* \qquad \text{....V-6}$$

Substitution of equation V-6 into equation V-4 defines a two point boundary value problem in x and λ as follows:

$$\frac{dx}{dt} = -x^2 - \lambda \quad ; \quad x(0) = 10 \qquad \text{....V-7}$$

$$\frac{d\lambda}{dt} = 2\lambda x - x \quad ; \quad x(1.0) = 0 \qquad \text{....V-8}$$

Solution yields x(t) and $\lambda(t)$ as is shown in Figure V-3. From V-6, $u^*(t)$ is immediately available. Solution of this problem is done off line. Analog, digital or hybrid methods may be used. A brief discussion of convenient techniques used will follow. References 1 through 5 consider solution to these problems in detail.

Off-Line Solution of the Two Point Boundary Value Problem

Digital: To solve problems such as that defined by equations V-7 and V-8, a trial and error technique must be used. This could be implemented

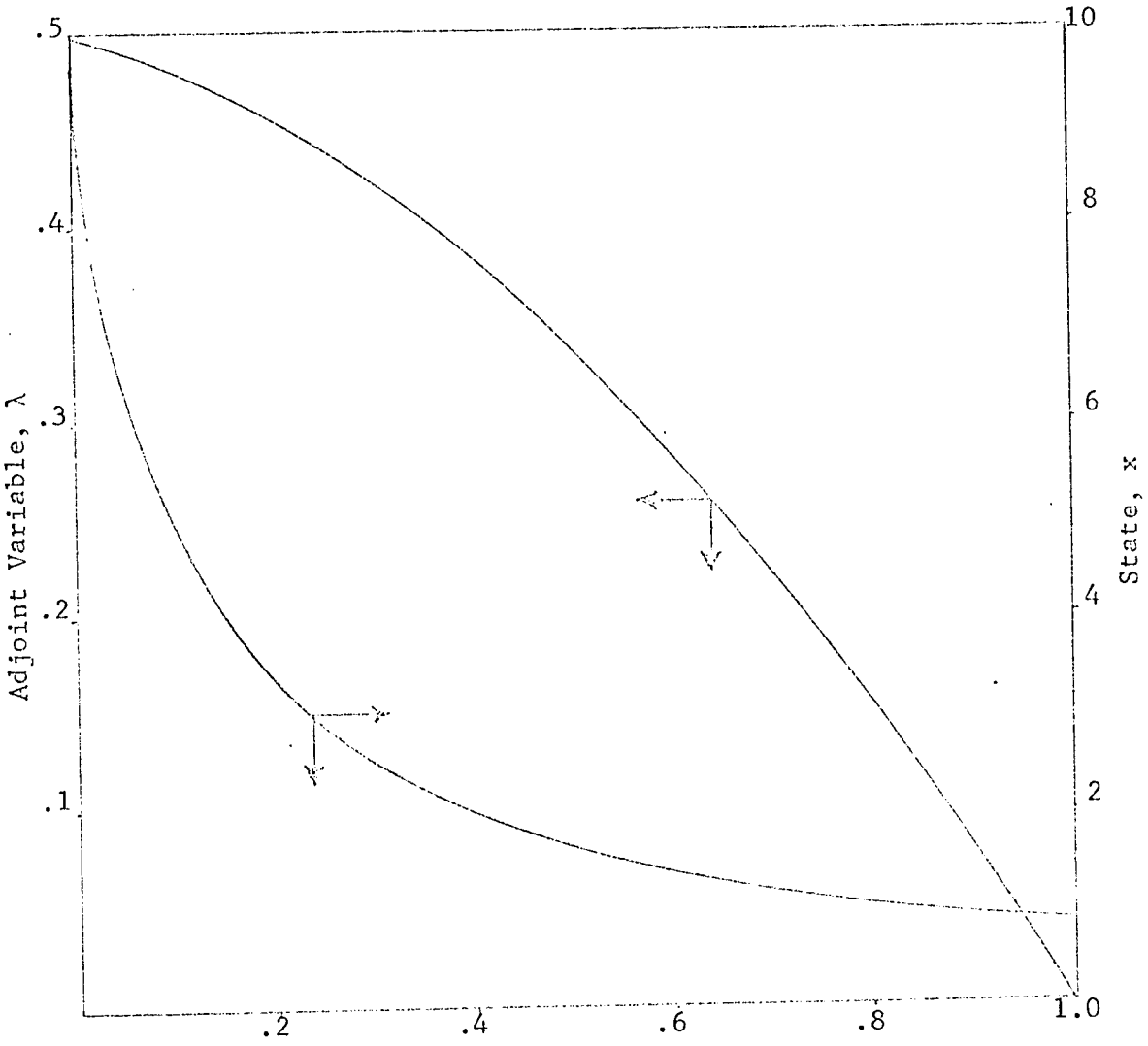


Figure V-3

Solution of Equations V-7, V-8

in either of two ways. First, the missing initial condition in equation V-8, λ, could be assumed and then forward integration of equations V-7 and V-8 would be carried out until $t = t_f$. At this point the final value of λ is compared with the boundary condition, e.g., $\lambda(t_f) = 0$. If these agree, we have the solution; if not, we must assume another $\lambda(t_o)$ and repeat the process.

The other possible trial and error process involves guessing the final value of the state variable, $x(t_f)$ and integrating equations V-7 and V-8 backward in time to t_o. At this point, $x(t_o)$ is compared with the initial boundary condition on x. If they agree, we have the correct solution; if not, we must guess another $x(t_f)$ and repeat the process. Multidimensional search techniques are useful for obtaining the trial values of the boundary conditions in an efficient way. An algorithm for such a solution will be illustrated in an example problem.

Although both procedures will work, the second method is by far the most practical to use, particularly in our case. The second procedure is referred to by Lapidus[1] as an approximation to the problem. This is because every trial generates an optimal control; however, it may be the optimal control for "another problem", defined by some other initial value of the state variable. This is just what we need since we want to resolve the problem for many values of the state variable at the various sampling points. The second procedure also has the advantage that the costate equation V-8 is usually more sensitive to the trial initial condition than is the state equation V-7 to a trial final condition.

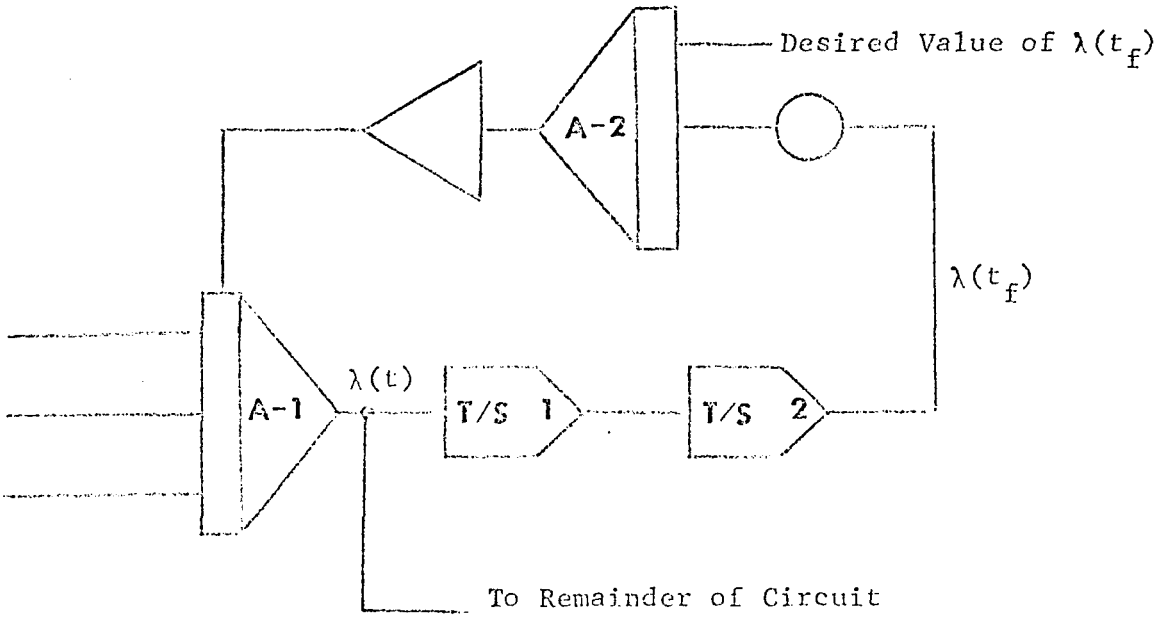
Analog: Boundary value problems such as equations V-7 and V-8 involving two first order equations can be handled conveniently on an analog computer with digital logic. This is done by operating in repetitive mode. The logic is set up such that the value of λ at t_f is compared to the actual desired value. The difference, or "error", is integrated and used as initial condition for the next integration of λ. A simplified analog diagram for this method is shown in Figure V-4.

Hybrid: Solution of two point boundary value problems may be carried out very rapidly on the hybrid computer. The procedure is the same as discussed above for digital solution except that the many trial integrations can be carried out much more rapidly on the analog computer.

Implementation of the Hybrid Controller

Our nonlinear system, equation V-1, was time scaled by a factor of ten so that the response time, t_f, is 10 seconds. This is faster than the dynamics of most process control loops. The hybrid controller was designed for sampling at four points along the state trajectory, t_s = 2, 4, 6, 8 seconds.

The two point boundary value problem, equations V-7 and V-8, was solved for ten different values of the state variable, x, at each sampling point. These values were chosen to surround the open loop optimal trajectory. The missing boundary conditions, λ, were obtained as a function of the chosen value of x. Typical curves of λ vs. x at



A-1 - Repetitive mode - Integrate - Initial Condition
TS-1 - Tracks when A1 is Integrating
TS-2 - Tracks when A1 is in Initial Conditions
A-2 - Integrates when A1 is in Initial Condition

Figure V-4

Analog Solution of Simple Two Point
Boundary Value Problem

different sampling points are shown in Figure V-5. Least squares regression was used to fit these curves to polynomial expressions. The average error in the resulting polynomials ranged from 0.087% to 0.50%. A typical polynomial for $t_s = 2$ is shown below:

$$\lambda = .2308 + .1431x - .0293x^2 + .00212x^3 \quad \ldots\ldots V\text{-}9$$

The nonlinear system was modeled on the analog computer as shown in Figure V-6. The analog portion of the hybrid controller is shown in Figure V-7. The digital program is shown in Appendix D.

Timing Considerations

As has been mentioned, the analog computer is capable of very fast integrations. For this problem, our two integrations needed to generate the optimal control from one sampling point to the next were executed in 0.02 seconds. During this 20 milliseconds, 50 points were sampled and stored as an array in the digital computer. This is a sampling rate of 2500 points/second. The array containing the optimal control is then transferred, point by point, back to the analog to control the system. The fifty points are transferred back in the two seconds between sampling points, or at a rate of 25 points/second.

Results

Figure V-8 shows the open loop optimal control. Figure V-9 illustrates the implementation of the hybrid controller for the case with

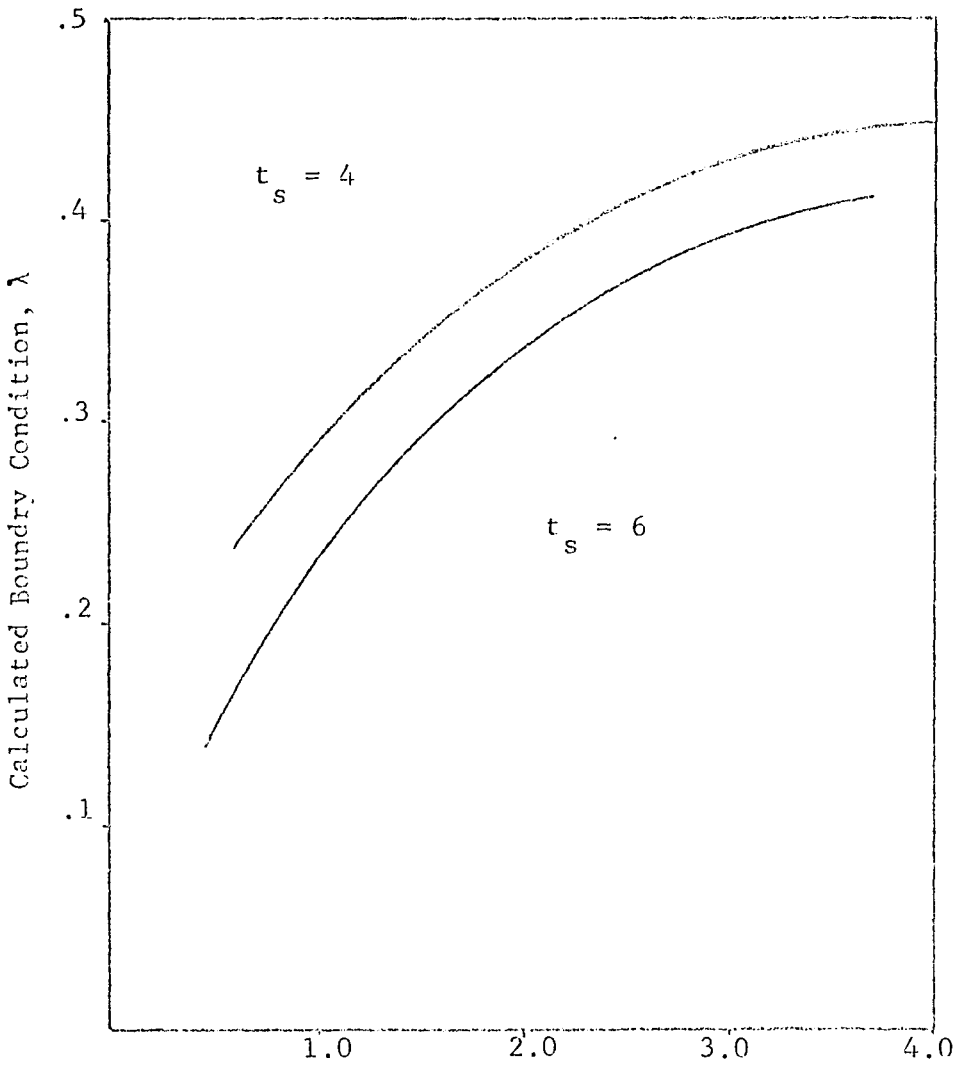

.5
.4
.3
.2
.1
Calculated Boundry Condition, λ
$t_s = 4$
$t_s = 6$
1.0
2.0
3.0
4.0
Sampled Value of State, X

Figure V-5

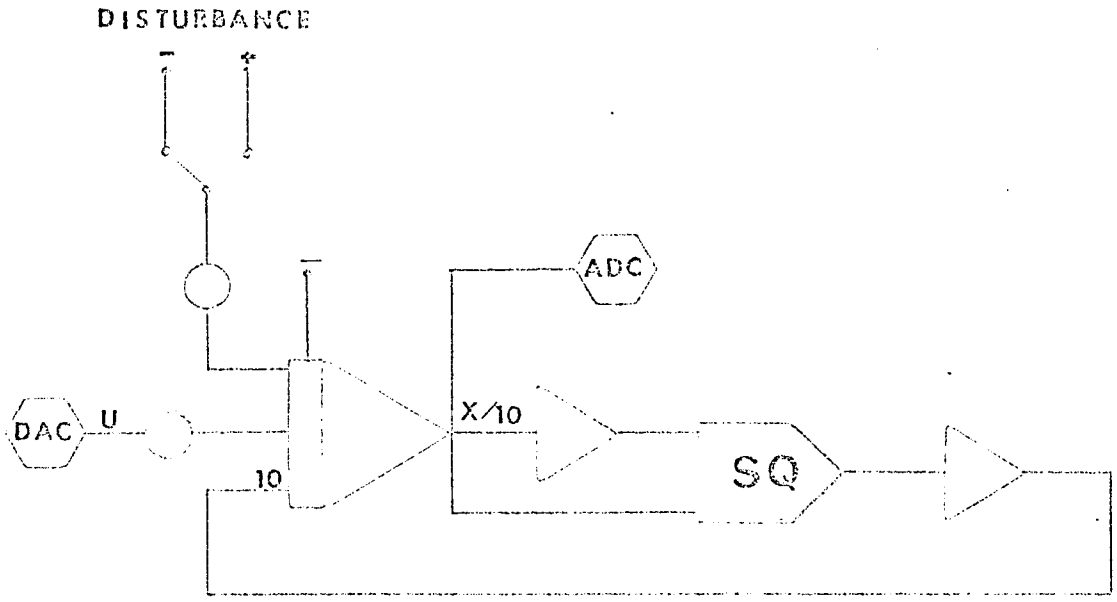


Figure V-6

Nonlinear System Model

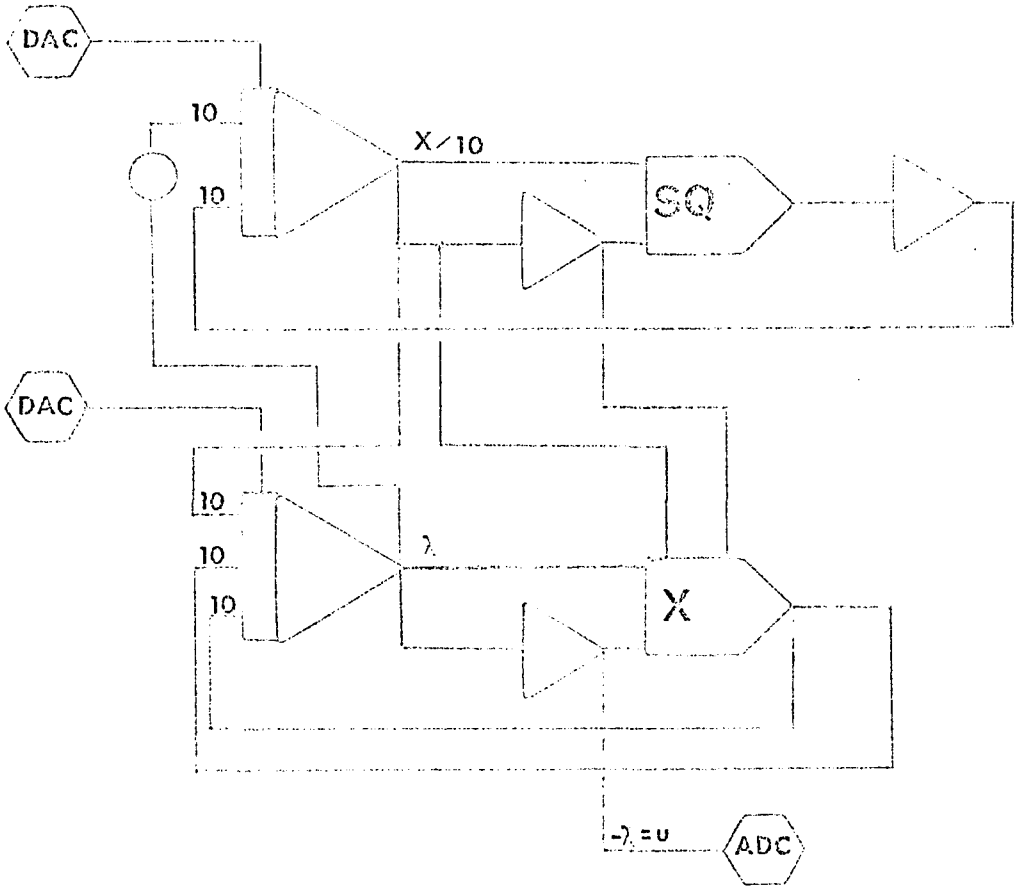


Figure V-7

Hybrid Controller

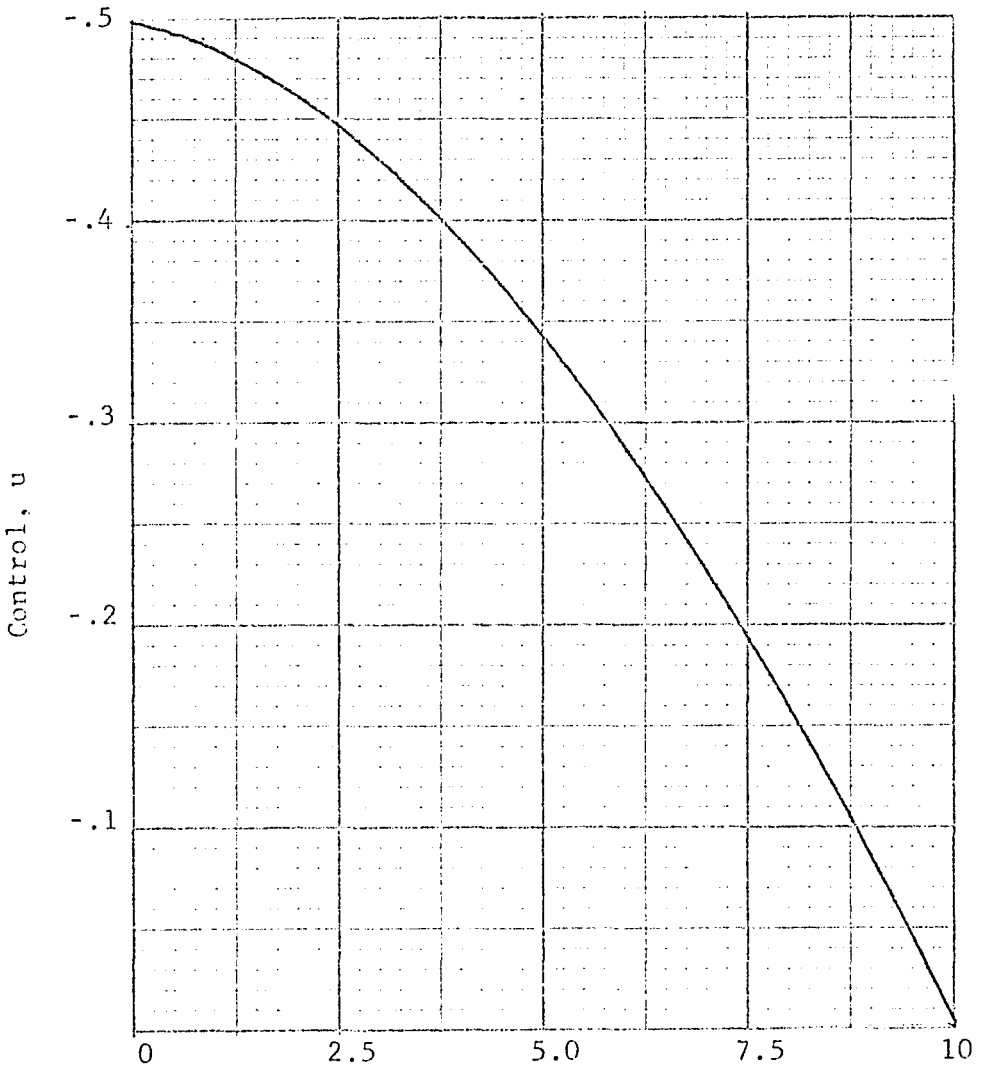


Figure V-8

Precalculated Open Loop Optimal Control

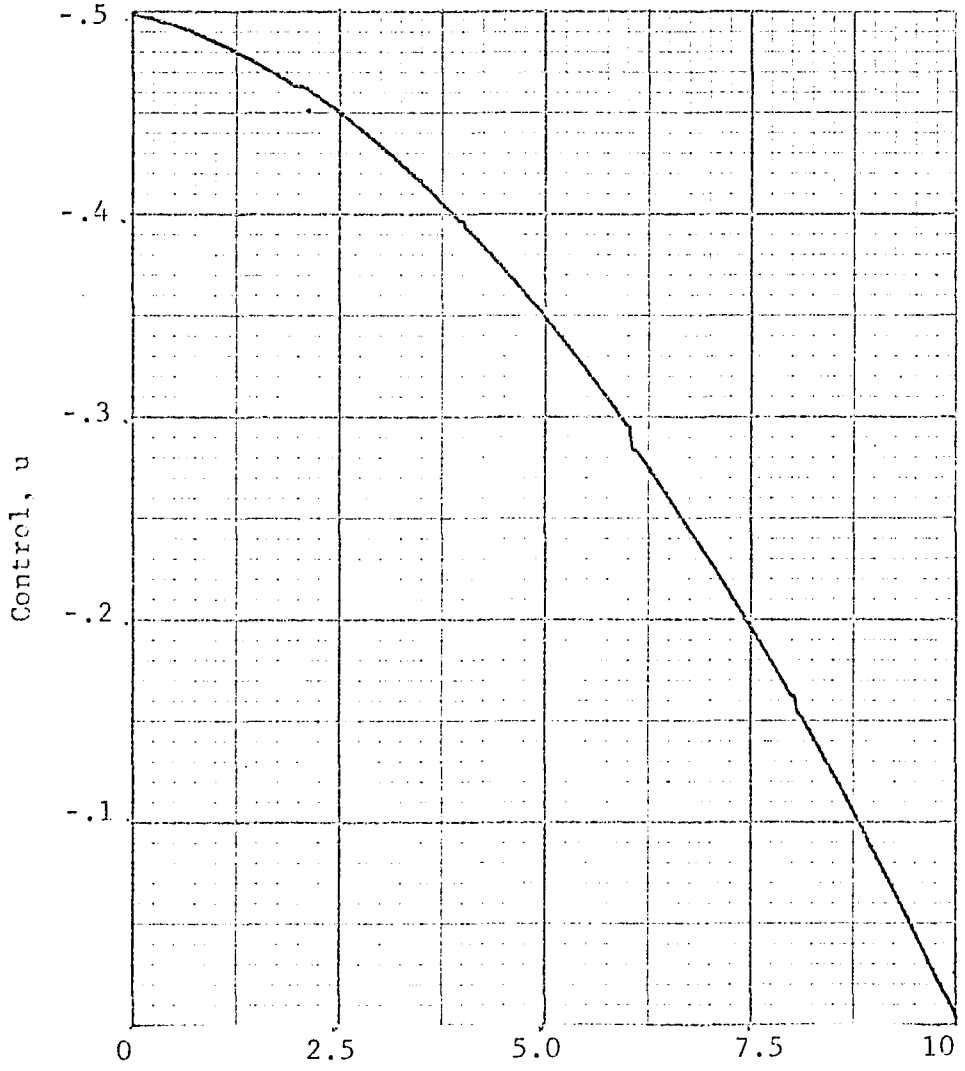


Figure V-9

Hybrid Control - No Disturbance

no disturbances. The slight discontinuities at the sampling points are due to slight errors in the polynomial equations.

Constant disturbances were added to the system at time equal to zero. Figure V-10 illustrates the control for various positive disturbances. Figure V-11 is the hybrid control action for various negative disturbances. Note that correction is made at each sampling point so that the control passes through the zero point. Figure V-12 is the resulting state trajectories for cases with the different disturbances entering the loop. Disturbances of -0.2, -0.4, +0.2, +0.4, +0.6 and +0.8 are shown in these figures.

To compare the hybrid feedback controller, the open loop (precalculated) optimal control was applied to the system and disturbances allowed to enter the loop. The cost, J, was calculated and compared to the cost obtained using the feedback hybrid controller. Table V-1 shows typical results.

Note that in every case as good or better control is obtained with the hybrid controller. In this example, however, the improvement is slight. This is due to the insensitivity of the control variable on the state variable.

Figure V-13 illustrates the improvement in the state trajectory by using the feedback hybrid control (as compared to the optimal open loop) for a constant disturbance of +0.6.

It is concluded from this simple example that the "hybrid controller" will provide an efficient means of obtaining closed loop

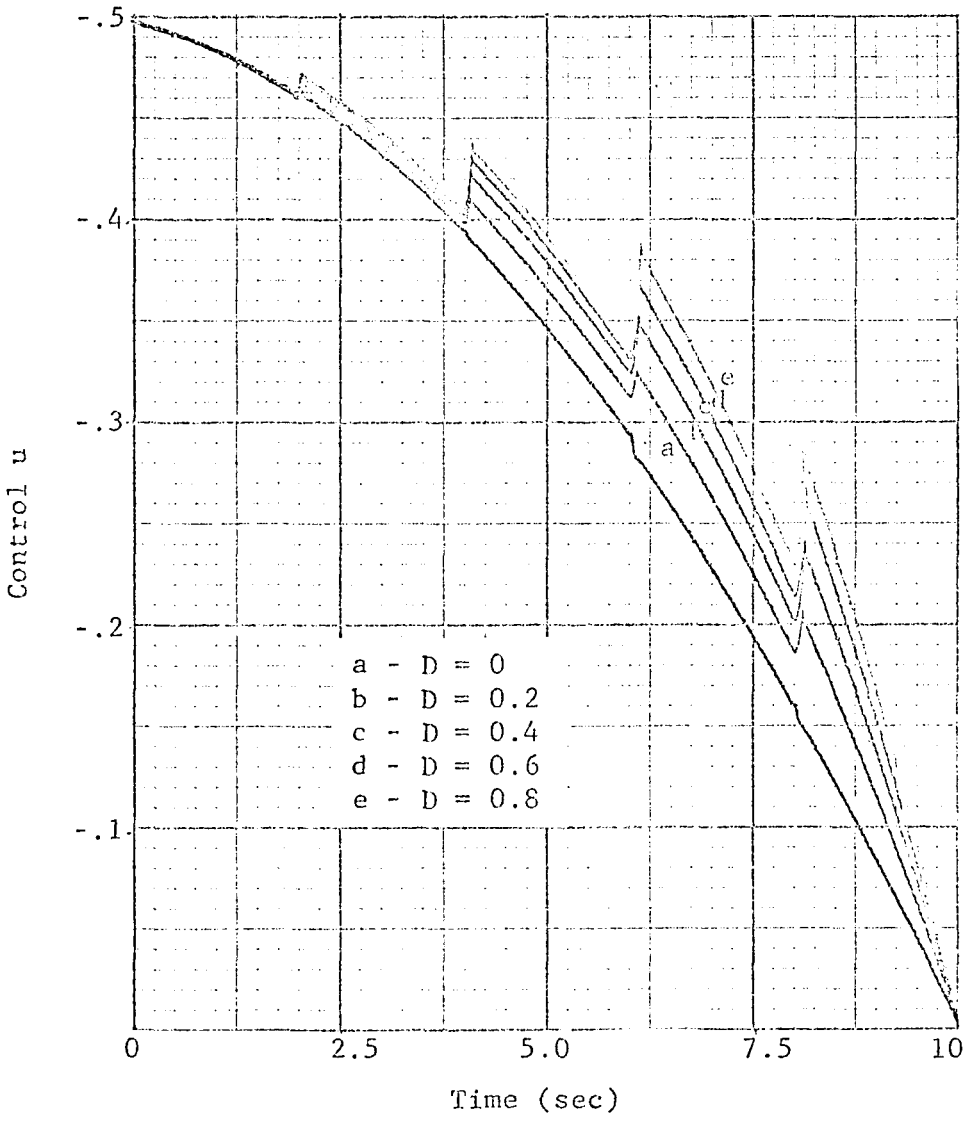


Figure V-10

Hybrid Control For Positive Disturbances

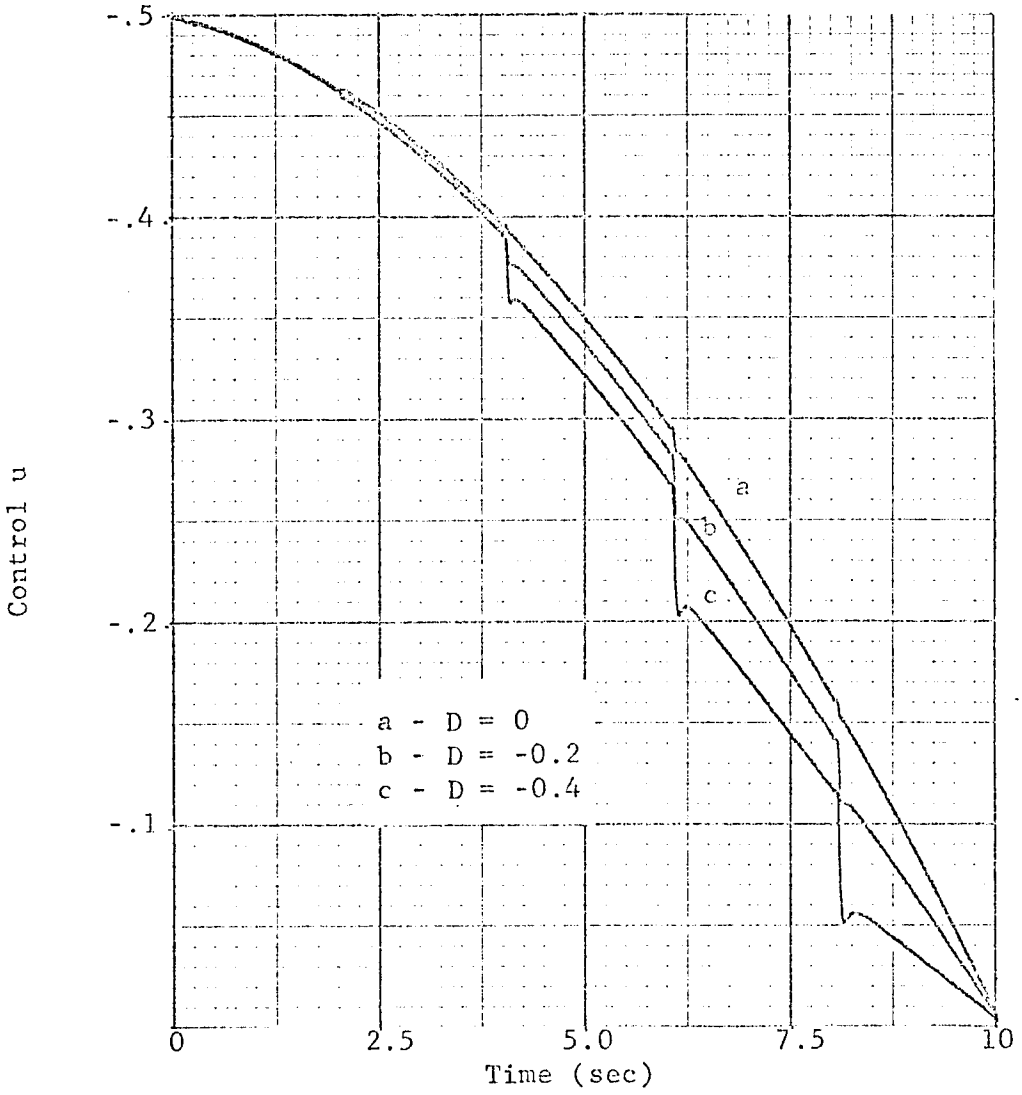


Figure V-11

Hybrid Control For Negative Disturbances

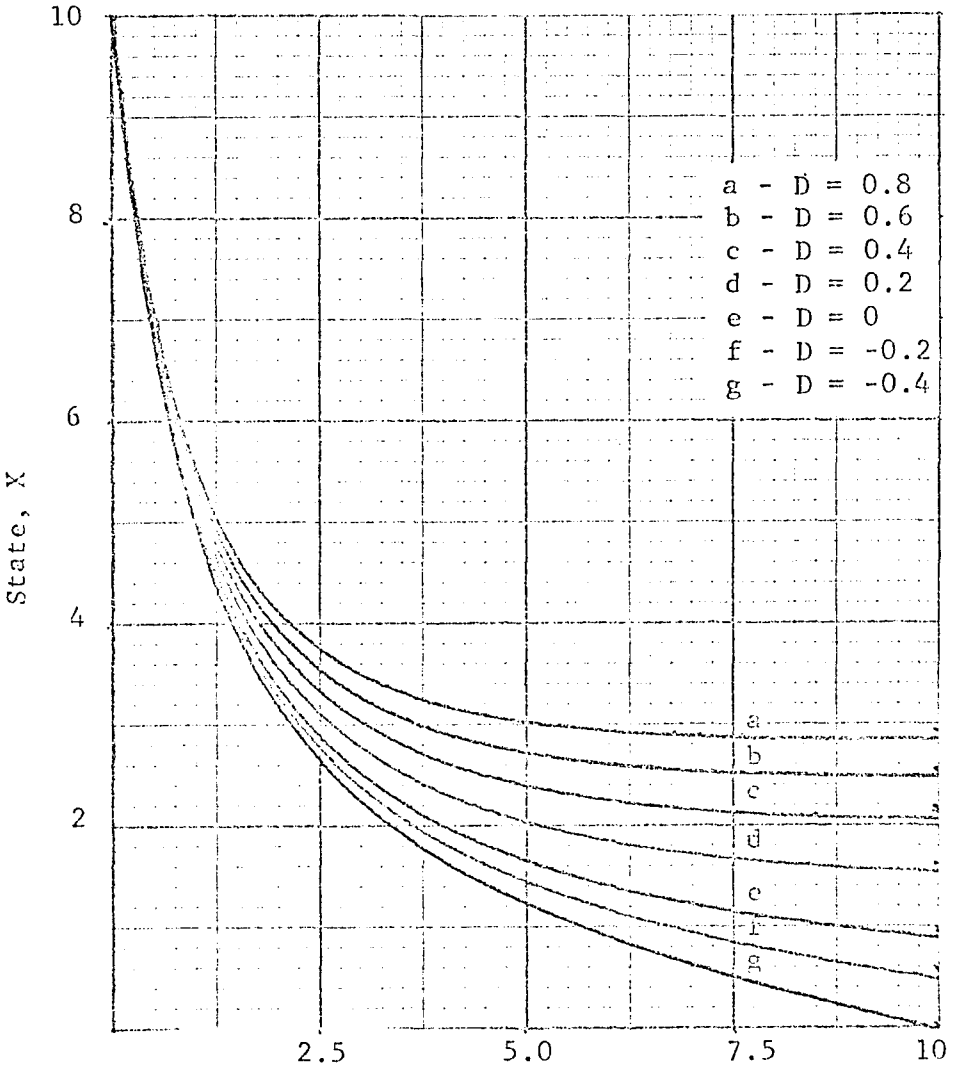


Figure V-12

State Trajectories for Various Disturbances

Table V-1

Cost Comparison Hybrid vs. Optimal Open Loop Controller

Disturbance	Optimal Open Loop	Hybrid
0.0	4.49	4.49
-0.2	5.16	5.16
-0.4	5.91	5.90
-0.6	6.69	6.68
-0.8	7.10	7.09
+0.2	3.97	3.96
+0.4	3.75	3.72

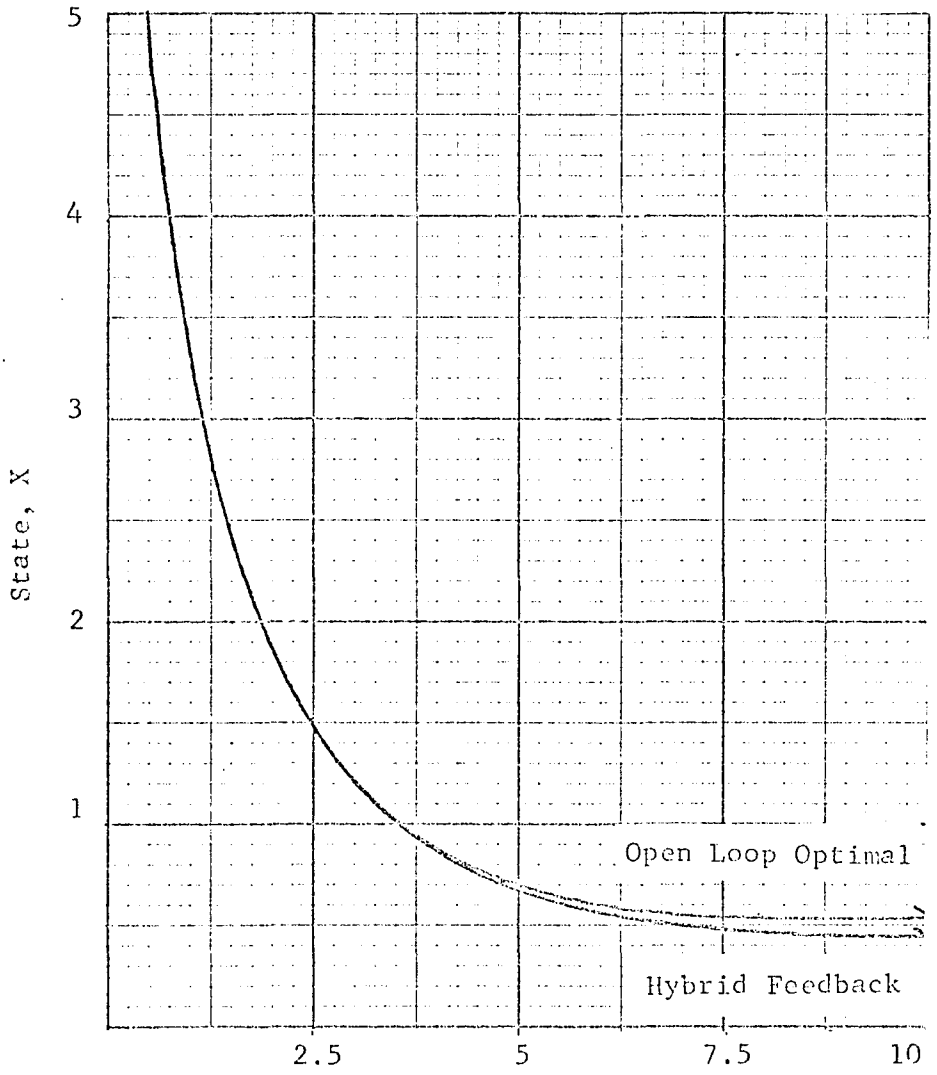


Figure V-13

Comparison of Optimal Open Loop and Hybrid Control

Constant Disturbance = 0.6

approximate optimal control for nonlinear systems.

One might immediately suspect that for more complicated systems this technique would not be practical due to the greater number of "off line" solutions needed and also the increased complexity of the integrations. To give this procedure a more difficult test, we will now consider a more complicated nonlinear system.

Hybrid Control of a Chemical Reactor

Consider the stirred tank chemical reactor illustrated in Figure V-14. This is similar to the system considered in Chapters III and IV. A second order reaction of the form:

$$2A \xrightarrow{k} B \qquad \text{....V-10}$$

is assumed to take place. The rate of reaction is expressed by:

$$\text{Rate} = -kC_A^2 \qquad \text{....V-11}$$

where C_A is the concentration of reactant A in the tank. The variation of rate constant, k, with temperature is expressed by an Arrhenius relationship as:

$$k = k_o \exp(-A/T) \qquad \text{....V-12}$$

where k_o is the frequency factor of the reaction, A is the activation

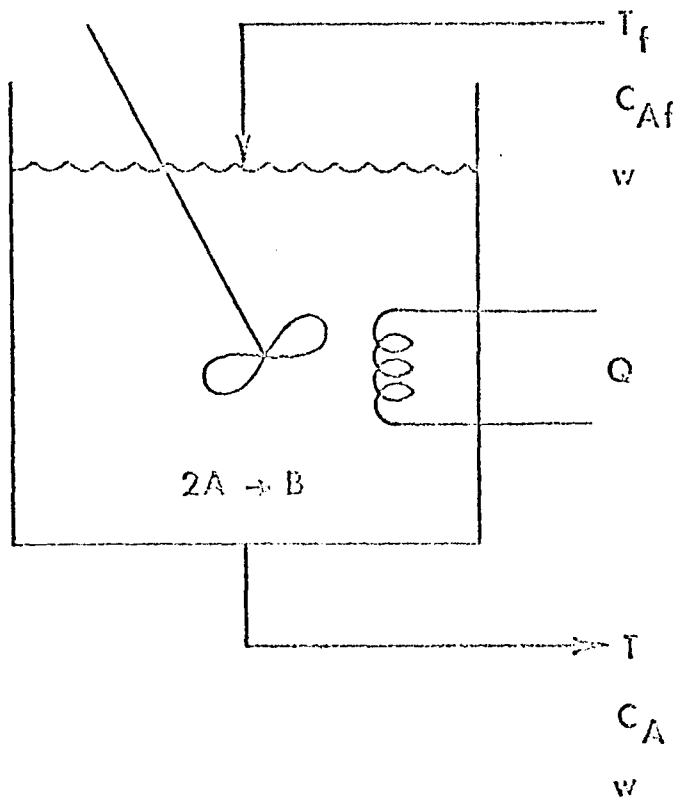


Figure V-14 Continuous Stirred-Tank Reactor

energy divided by the gas constant and T is absolute temperature.

The problem is to control the heat transfer, Q, in such a way that the following performance criterion is minimized:

$$J = \int_0^{t_f} (C_A^2 + bQ^2)\,dt \qquad \ldots.V\text{-}13$$

where t_f is the specified final time and b is a constant. For this example, let there be:

$$t_f = 10 \text{ min.}$$

$$b = 10^{-10}$$

The reactor is modeled by mass and energy balances. The unsteady state mass balance on component A yields:

$$\frac{dC_A}{dt} = \frac{W}{V\rho}(C_{Af} - C_A) - kC_A^2 \qquad \ldots.V\text{-}14$$

where W is the inlet flow rate, V is the tank volume, ρ is the density of the material in the tank, and C_{Af} is the concentration of the feed.

The unsteady state energy balance on the reactor yields:

$$\frac{dT}{dt} = \frac{W}{V\rho}(T_f - T) + \frac{Q}{V\rho C_p} - \frac{\Delta H k C_A^2}{V\rho C_p} \qquad \ldots.V\text{-}15$$

where T_f is the feed temperature, C_p is the average heat capacity of the

contents of the reactor, and ΔH is the heat of reaction for the exothermic reaction.

The system parameters are assumed to be:

$$C_p = 0.90 \text{ Btu/lb } ^{\circ}F$$
$$V = 250 \text{ ft}^3$$
$$\rho = 60 \text{ lb/ft}^3$$
$$A = 2560^{\circ}R$$
$$\Delta H = -867 \text{ Btu/lb A}$$
$$k_o = 1.425 \text{ ft}^3/\text{lb min.}$$

Steady state operating conditions are:

$$T = 190^{\circ}F$$
$$k = .0278 \text{ ft}^3/\text{lb min.}$$
$$W = 1000 \text{ lb/min.}$$
$$T_f = 150^{\circ}F$$
$$C_{Af} = 9.0 \text{ lb/ft}^3$$

The problem is set up so as to "start-up" the reactor in such a way as to minimize J. Hence, the initial concentration and temperature will be specified as the feed conditions:

$$C_A(t_o) = 9.0 \text{ lb/ft}^3$$
$$T(t_o) = 150^{\circ}F$$

Application of the Maximum Principle

Now that the system is specified, we can define the necessary conditions for an optimal open loop control policy, $Q^*(t)$. The Hamiltonian may be written as:

$$H = C_A^2 + bQ^2 + \lambda_1\left[\frac{W}{V\rho}(C_{Af}-C_A)-kC_A^2\right] + \lambda_2\left[\frac{W}{V\rho}(T_f-T)+\frac{Q}{V\rho C_p}-\frac{\Delta Hk C_A^2}{V\rho C_p}\right] \quad \ldots.V\text{-}16$$

The necessary conditions for an extremal are:

$$\frac{dC_A}{dt} = \frac{W}{V\rho}(C_{Af}-C_A) - kC_A^2 \quad \ldots.V\text{-}17$$

$$\frac{dT}{dt} = \frac{W}{V\rho}(T_f-T) + \frac{Q}{V\rho C_p} - \frac{\Delta Hk C_A^2}{V\rho C_p} \quad \ldots.V\text{-}18$$

$$\frac{d\lambda_1}{dt} = -\frac{\partial H}{\partial C_A} = -2C_A + \frac{\lambda_1 W}{V\rho} + 2\lambda_1 kC_A + \frac{2\lambda_2 \Delta Hk C_A}{V\rho C_p} \quad \ldots.V\text{-}19$$

$$\frac{d\lambda_2}{dt} = -\frac{\partial H}{\partial T} = \lambda_1 \frac{a}{T^2}k + \frac{\lambda_2 W}{V\rho} + \frac{\lambda_2 \Delta Hak C_A^2}{V\rho C_p T^2} \quad \ldots.V\text{-}20$$

$$\frac{\partial H}{\partial Q} = 0 = 2bQ^* + \frac{\lambda_2}{V\rho C_p} \quad \ldots.V\text{-}21$$

Solving equation V-21 for Q^* yields:

$$Q^*(t) = -\lambda_2/(2V\rho C_p b) \quad \ldots.V\text{-}22$$

Substitution of equation V-22 into equation V-18 yields:

$$\frac{dT}{dt} = \frac{W}{V\rho}(T_f - T) - \frac{\lambda_2}{2b(V\rho C_p)^2} - \frac{\Delta H k C_A^2}{V\rho C_p} \quad \ldots\ldots V\text{-}23$$

Equations V-17, V-23, V-19 and V-20 now define our two point boundary value problem. The boundary conditions are:

$$C_A(t_o) = 9.0 \text{ lb/ft}^3$$
$$T(t_o) = 150^{\circ}F$$
$$\lambda_1(t_f) = 0$$
$$\lambda_2(t_f) = 0$$

where: $t_o = 0$

$t_f = 10$ min.

Notice that solution of these equation is considerably more complicated than the two differential equations defined by our first order example. Not only have the number of equations (and missing boundary conditions) increased but also degree of nonlinearity has also increased. Remember that k is an exponential function of temperature.

"Off Line" Solution

The "off line" solution of these equations is handled on the digital computer by the "approximation to the problem" method previously discussed. The final values of concentration, C_A, and temperature, T,

are assumed. Equations V-17, V-23, V-19 and V-20 are then integrated backward and the resulting temperature and concentration are compared with the known values. If they agree, we have the solution; if not, new final values are assumed. A multivariable pattern search[6] technique is used to obtain the new values. This is done by minimizing the differences between the desired initial values and those actually obtained. This is done by minimizing the following cost function:

$$\text{Cost} = (C_{AD}-C_A^i)^2 + (T_D-T^i)^2$$

C_{AD} and T_D are the desired concentration and temperature (initial conditions). C_A^i and T^i are the initial values obtained on the ith guess of the final values of C_A and T. This procedure is illustrated diagrammatically in Figure V-15. The Fortran program for the solution is presented in Appendix D.

As in the first example, we desire to obtain a table of λ_1 and λ_2 as functions of the state variables, C_A and T. This table must be generated at each sampling point. Since in this case we have two state variables, we must perform this off line solution at more points surrounding our trajectory. That is, to obtain a meaningful relationship between the variables, we must hold one constant and vary the other independently.

Off line solutions were carried out in a factorial design. Five temperature points were chosen that surround the precalculated temperature trajectory. At each of these points five concentration levels were used

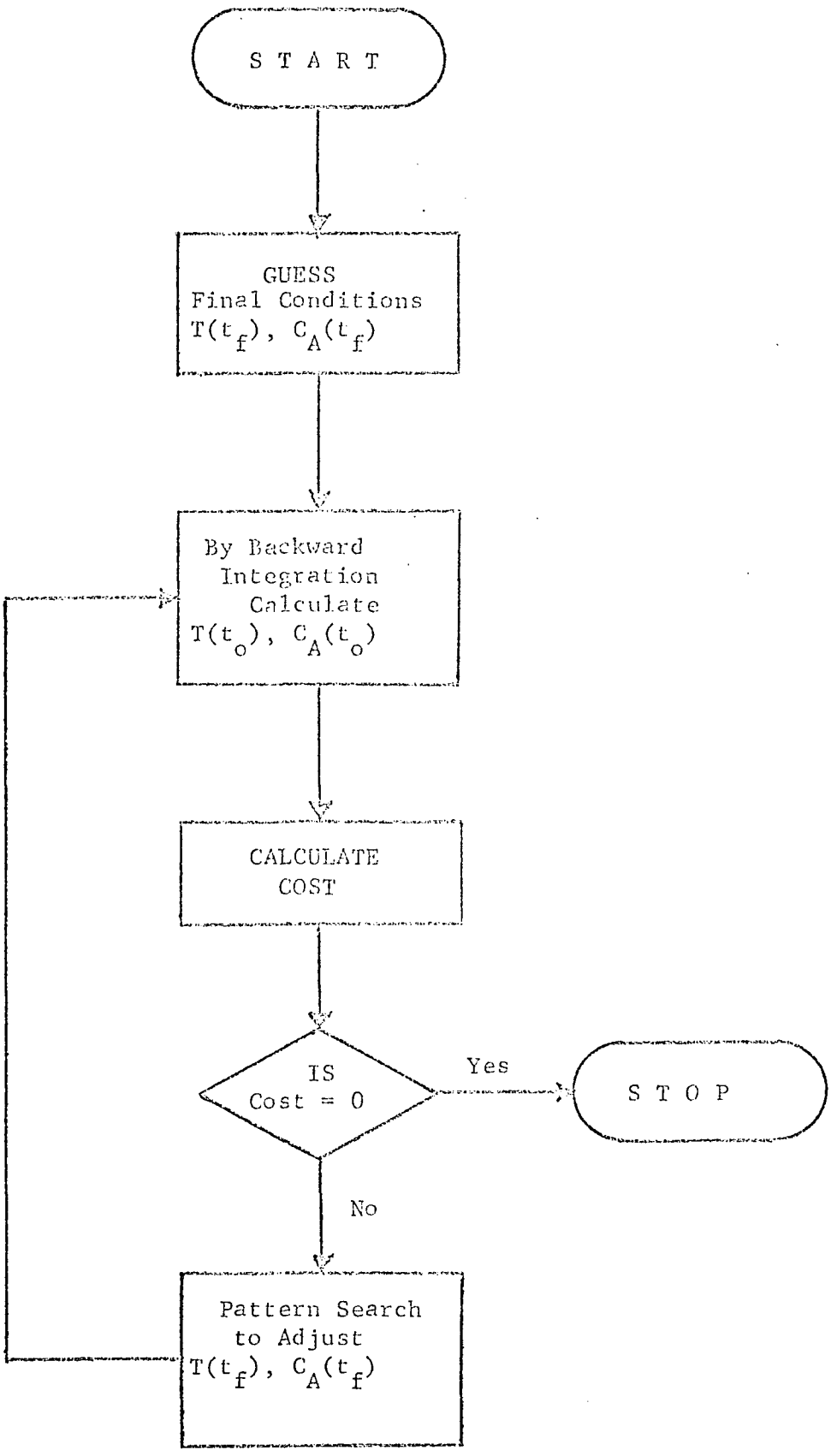


Figure V-15
Algorithm For Digital Solution of Two Point Boundary Value Problem

that surround the precalculated optimal concentration trajectory. Therefore twenty-five solutions were obtained for each sampling point. Typical results of these solutions are shown in Table V-2 for a final time of 8 min. (i.e., sampling after 2 minutes).

From the table of solutions (λ_1 and λ_2 vs. T and C_A), polynomials were obtained for λ_1 and λ_2 as functions of T and C_A. A stepwise multiple regression program[7] was used for obtaining these polynomials. Excellent fits were obtained in every case. Multiple correlation coefficients ranged from 0.996 to 1.0. The standard error of the estimates was always smaller than 1%. Typical resulting polynomials are shown below for $t_f = 6$:

$$\frac{\lambda_1 x 10^4}{500} = 19.96 + 1702.7C - 1.958CT \qquad \text{....V-24}$$

$$\lambda_2 x 10^4 = 144.81 + 159.95C - .124CT \qquad \text{....V-25}$$

where the factors 10^4 and 500 are for scaling purposes.

Hybrid Simulation

The controller was designed for sampling at four points, $t_s = 2$, 4, 6 and 8 min. Simulation of the reactor was done on the analog computer and is shown in Figure V-16. Table V-3 shows the potentiometer assignment sheet.

Note that the exponential term in the rate constant is generated

Table V-2

Off Line Solutions for t_f = 8 min.

Temp.($^{\circ}$R)	Concentration (lb/ft^3)	λ_1(500)	λ_2
610	8	.4303	.1079
	7	.3772	.0991
	6	.3256	.0912
	5	.2749	.0796
	4	.1808	.0707
620	8	.4106	.1042
	7	.3607	.0967
	6	.3115	.0872
	5	.2634	.0792
	4	.2177	.0695
630	8	.3931	.1035
	7	.3453	.0967
	6	.2986	.0881
	5	.2530	.0788
	4	.2098	.0692
⋮	⋮	⋮	⋮

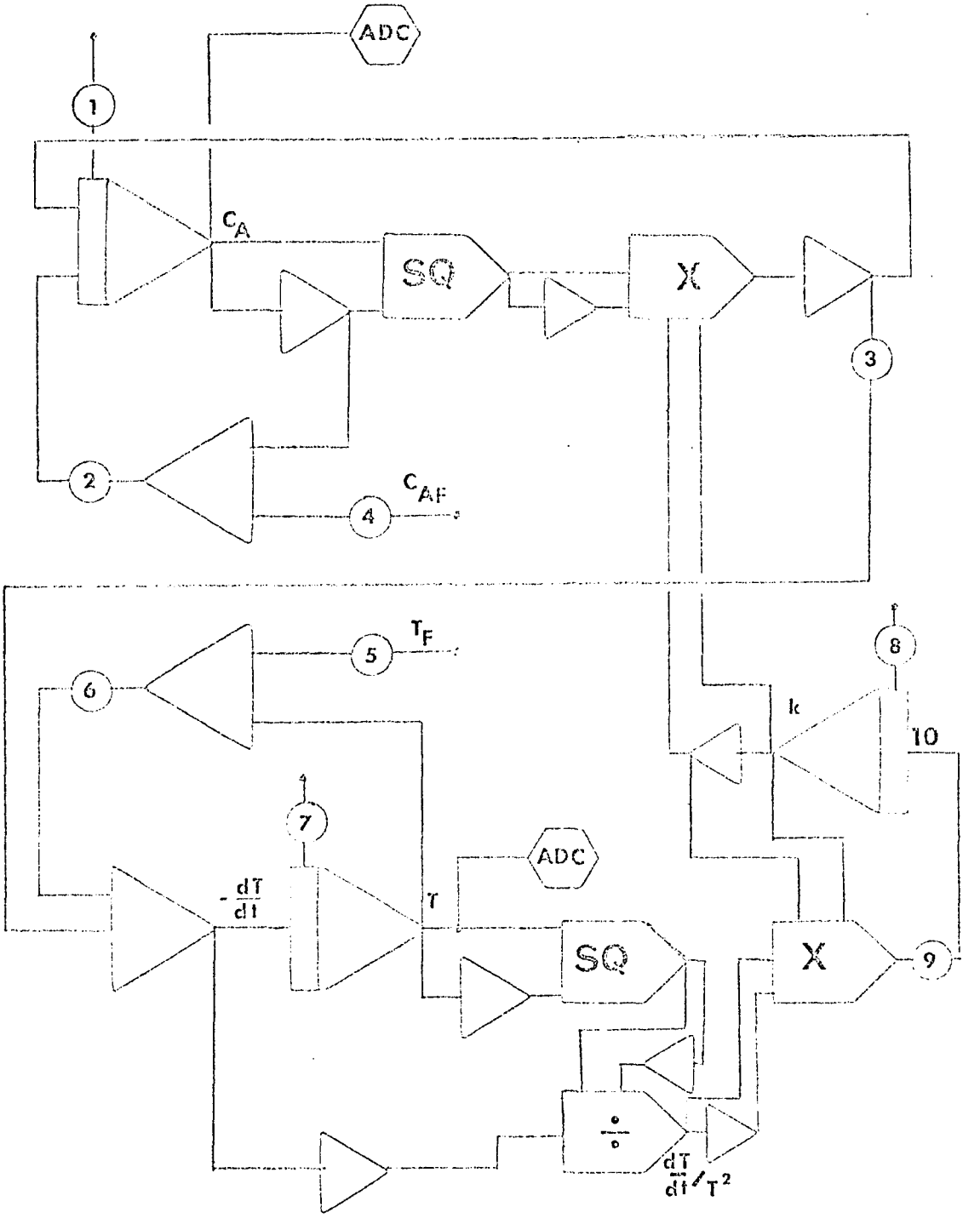


Figure V-16

Reactor Model

Table V-3

Potentiometer Assignment* Sheet for Reactor Simulation

Potentiometer Number	Function†	Setting
1	$C_A(t_o)/10$	0.9000
2	$W/V\rho$	0.0667
3	$\Delta H/100V\rho C_p$	0.0006
4	$C_{AF}/10$	0.9000
5	$T_F/1000$‡	0.6100
6	$W/V\rho$	0.0667
7	$T(t_o)/1000$	0.6100
8	$10k(t_o)$	0.2139
9	$a/10^4$	0.2560

*Potentiometer numbers correspond to those in Figure V-16 and not actual potentiometer numbers on EAI-680 Board.

†Magnitude scaling can be determined from initial condition potentiometers.

‡Temperature is in ^oR.

by observing that:

$$\frac{dk}{dt} = \frac{dk}{dT} \cdot \frac{dT}{dt} \qquad \text{....V-26}$$

Solving for $\frac{dk}{dT}$ yields:

$$\frac{dk}{dT} = k_o \frac{A}{T^2} e^{-A/T} = k \frac{A}{T^2} \qquad \text{....V-27}$$

Therefore:

$$\frac{dk}{dt} = k \frac{A}{T^2} \frac{dT}{dt} \qquad \text{....V-28}$$

The control strategy is obtained by the analog solution of equations V-17, V-23, V-19 and V-20. The initial conditions for λ_1 and λ_2 are transferred from the digital computer memory prior to the start of the integration. The sampled values of the temperature and concentration are also transferred from the digital computer and used as initial conditions. Figure V-17 illustrates the analog hardware. Note that an initial value of k must be transferred to the analog along with the sampled value of T. This is because the integration of equation V-28 must have an initial condition and it must be compatable with the initial condition on T if the implicit generation k is to be correct. This can be done conveniently by

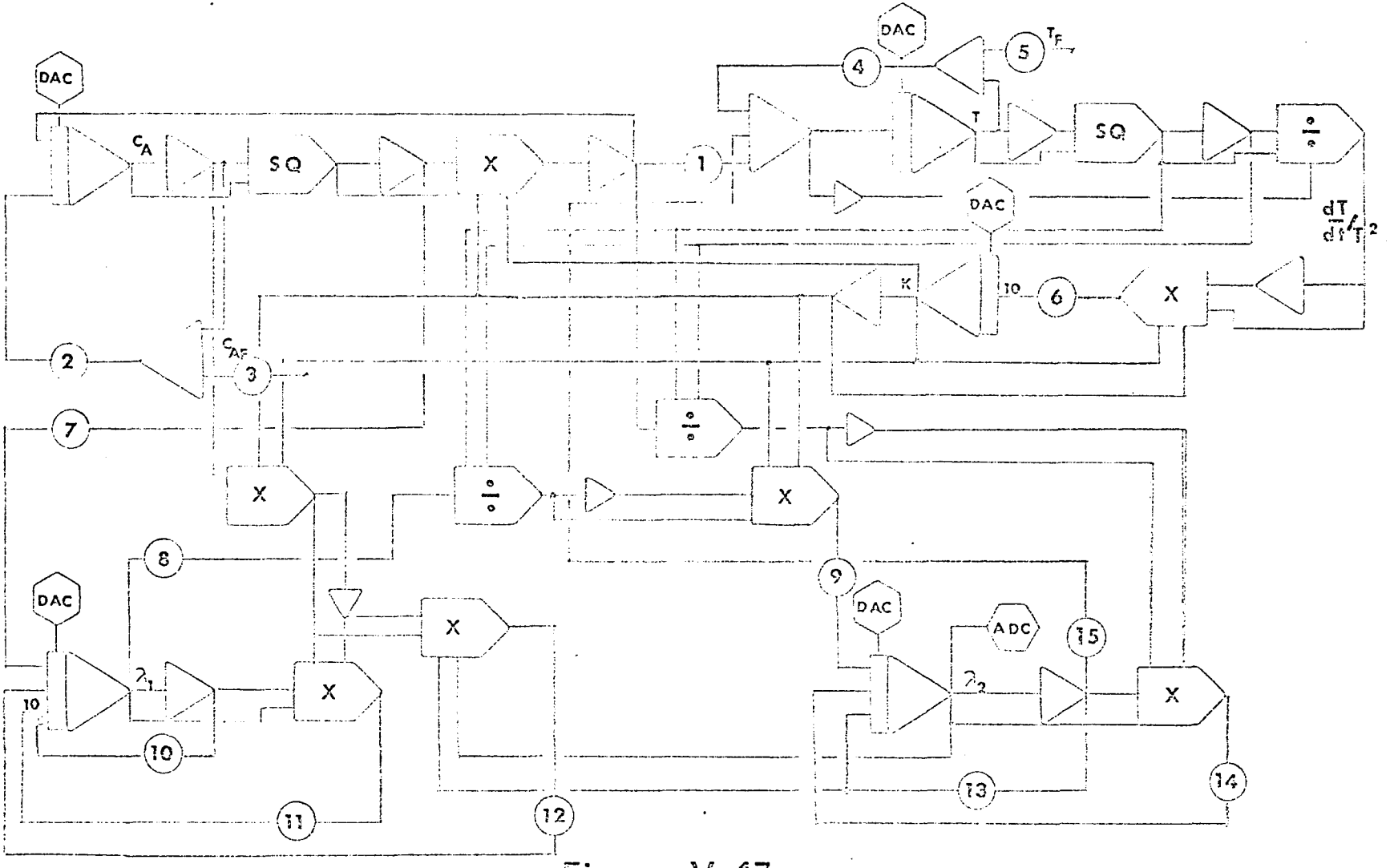


Figure V-17

Hybrid Controller

digital calculation of the value of k corresponding to the sampled value of T. This calculated value of k is transferred back to the analog with the other initial conditions. Table V-4 shows the potentiometer assignment and magnitude scaling.

Timing

The system was time scaled by a factor of 60 so that the response covered 10 seconds and not 10 minutes.

This, of course, put a greater strain on the controller since faster calculation of optimal control was required. The analog part of the controller operates 100 times faster than the system. Therefore, calculation of the control for the two seconds between sampling is done in .02 seconds. During this .02 seconds, fifty points are sampled and stored in the digital computer memory for use in controlling the system.

Results

Figure V-18 shows the analog solution to equations V-17 and V-23. This is the temperature and concentration response with the optimal control or Q added to the system. No disturbance is present. This solution, $C_A(t)$ and $T(t)$, is used to obtain the surrounding points for the "off line" solutions mentioned previously. Figure V-19 shows the corresponding solutions to equations V-19 and V-20 for the costate variables, λ_1 and λ_2. Recall that Q is related to λ_2 through

Table V-4

Potentiometer Assignment* Sheet for Hybrid Control of Reactor

Potentiometer Number	Function†	Setting
1	$\Delta H/V\rho$	0.0642
2	$W/V\rho$	0.0667
3	$C_{AF}/10$	0.9000
4	$W/V\rho$	0.0667
5	$T_F/1000$‡	0.610
6	$a/10^4$	0.2560
7	Scale (2/5)	0.4000
8	Scale (1/2)	0.5000
9	$2x5a/10^5$	0.2560
10	$W/V\rho$	0.0667
11	Scale (2/10)	0.0200
12	$2\Delta H/500V\rho C_p$	0.0003
13	$W/V\rho$	0.0667
14	$\Delta Ha/V\rho C_p 10^5$	0.0016
15	$1000(V\rho C_p)^2 b/2$	0.0274

*Potentiometer numbers correspond to those in Figure V-17 and not actual potentiometer numbers on EAI-680 Board.

†Magnitude scaling can be determined from initial condition potentiometers.

‡Temperature is in ^{o}R.

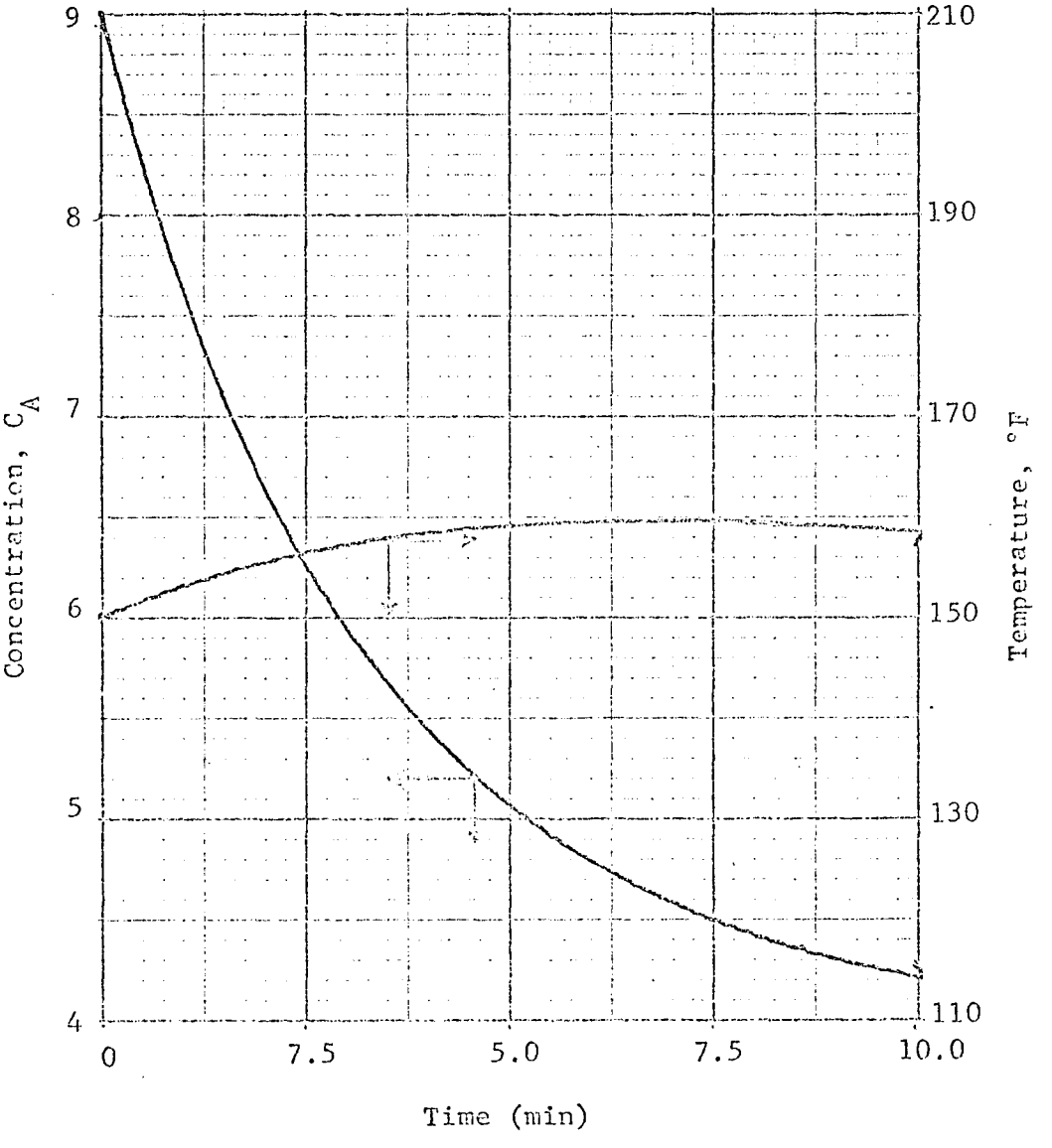


Figure V-18

Analog Open Loop Solution:
Concentration and Temperature Response

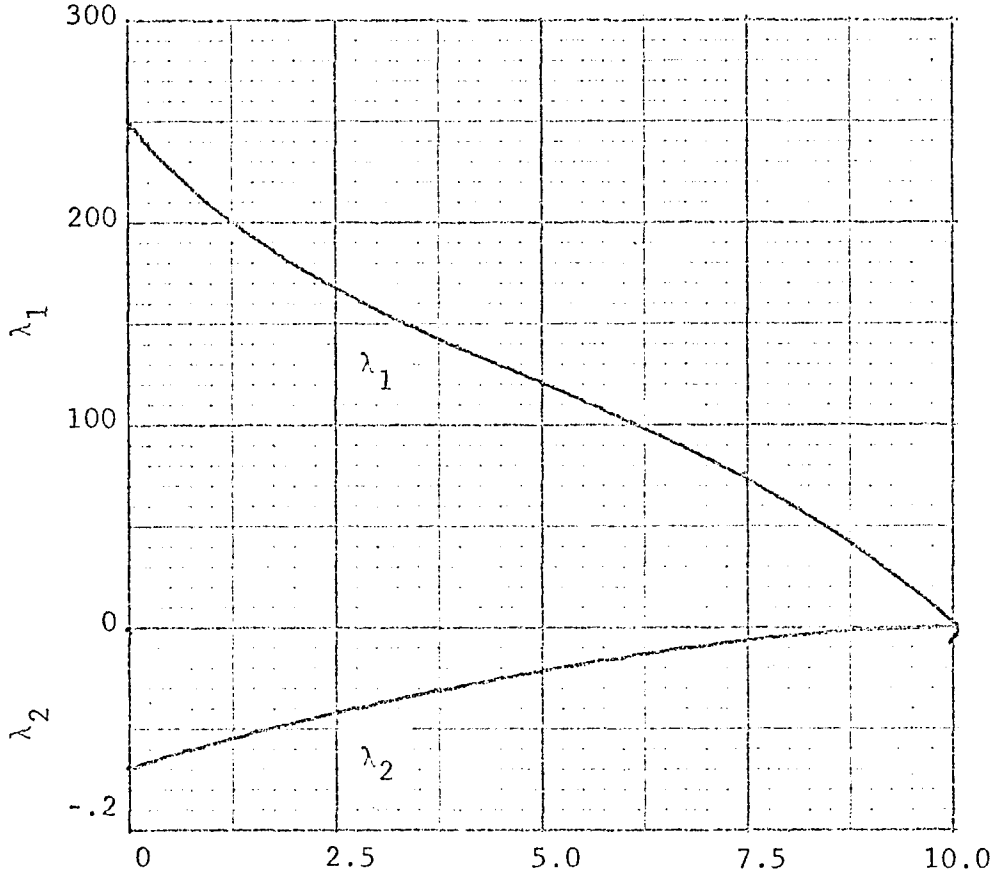


Figure V-19

Analog Open Loop Solution: λ_1, λ_2 vs Time

equation V-21. Therefore generation of $\lambda_2(t)$ yields Q(t).

Figure V-20 shows the implementation of the hybrid controller for the case with no disturbances. Note the slight discontinuity at the sampling points. This is due to the slight inaccuracies in the polynomial equations. Note that Q must go to zero at t_f = 10 min. since λ_2 goes to zero.

Using the hybrid controller λ_1 starts at 245 and ends at 1.5. This slight deviation from the optimal analog solution (245 to 0) is also due to the deviations in the polynomial equations.

To test the closed loop or feedback nature of the hybrid controller, various disturbances were put into the system. Changes in feed concentration and temperature were made. In practice, such "typical" disturbances could be anticipated and accounted for in the design of the controller. The feed concentration and temperature could be measured and correction for upset made prior to its effort on the output concentration and temperature. This would be a "feedforward" control loop. For this example, however, it will be assumed that there was no way to anticipate such upsets and their effect can only be known by the effect on the output variables.

Figures V-21 through V-23 show the effect of changes in feed concentration. Figure V-21 is the concentration response. Figure V-22 shows the various temperature responses. As would be expected, the effect (on the concentration response) is greater. C_{Af} equal nine in these figures corresponds to the no disturbance. As the system was

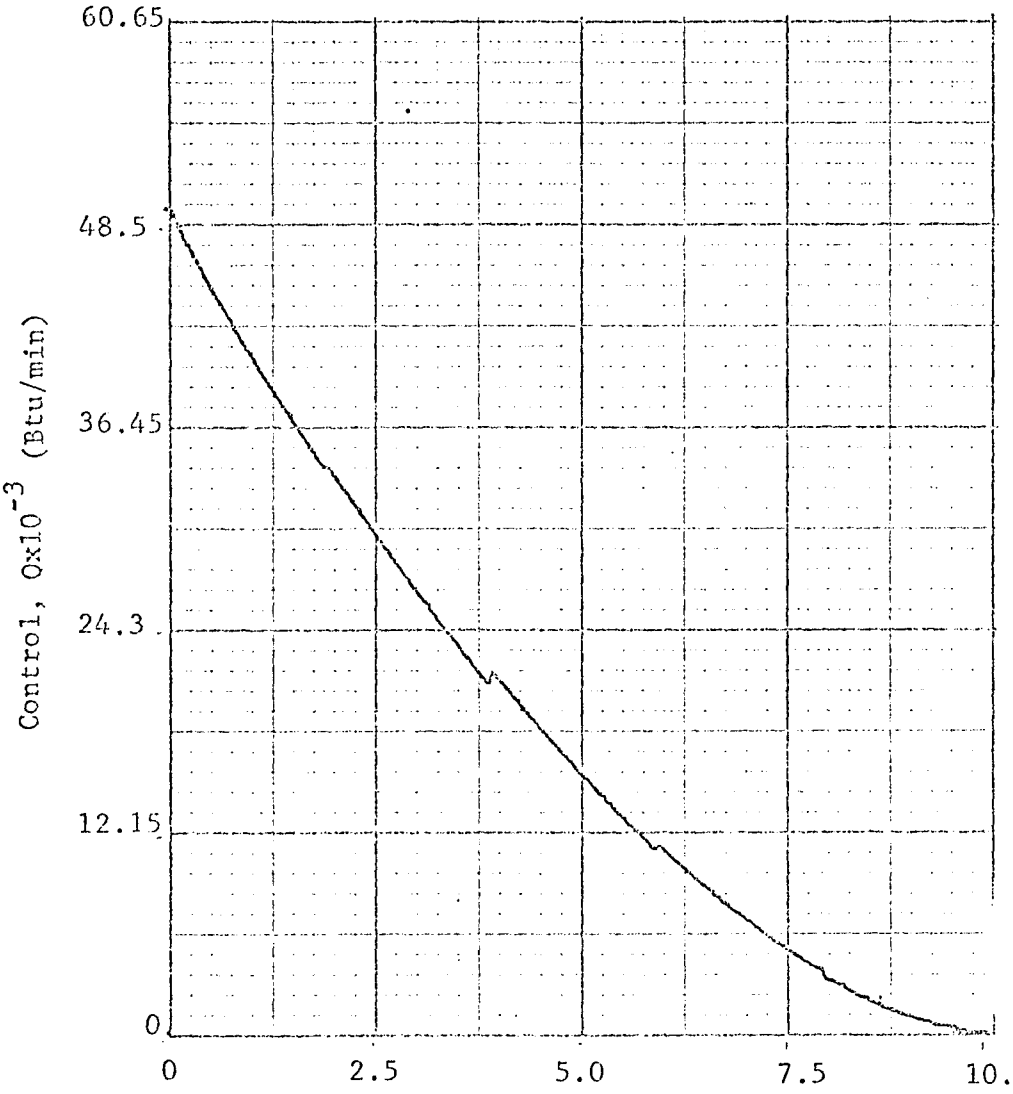


Figure V-20

Hybrid Control For No Disturbance

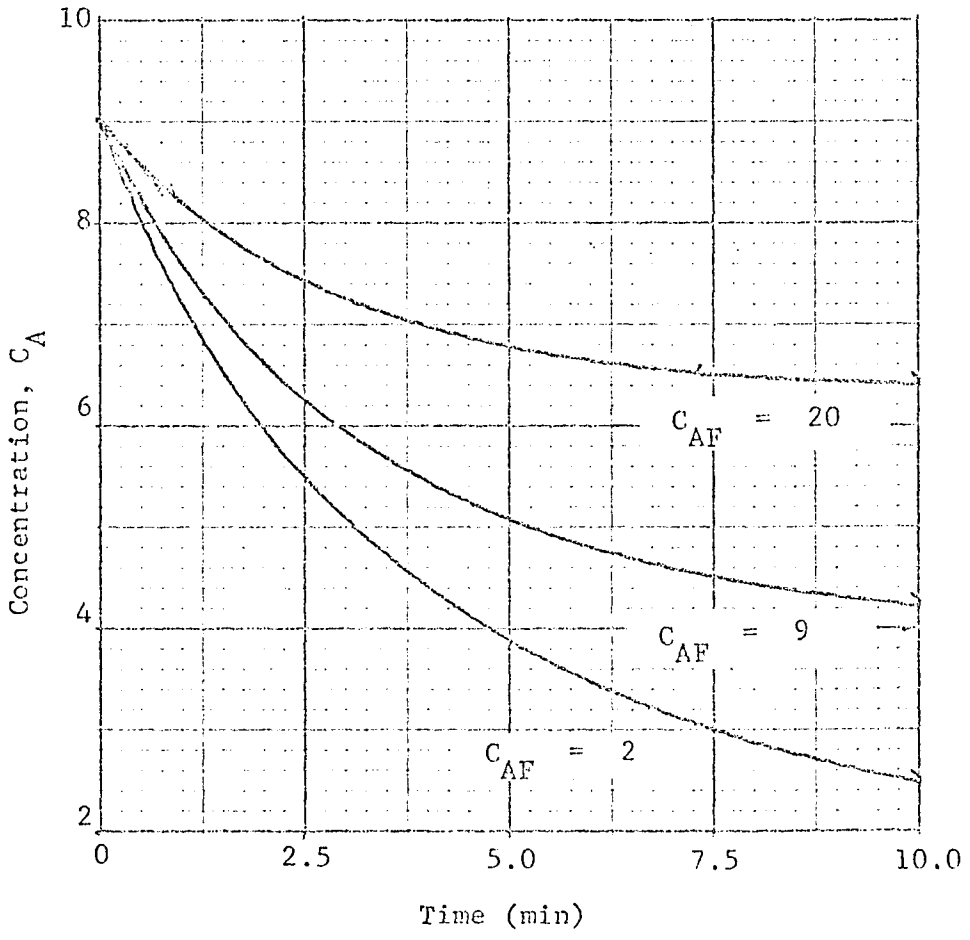


Figure V-21

Concentration Response for
Constant Disturbances in
Feed Concentration

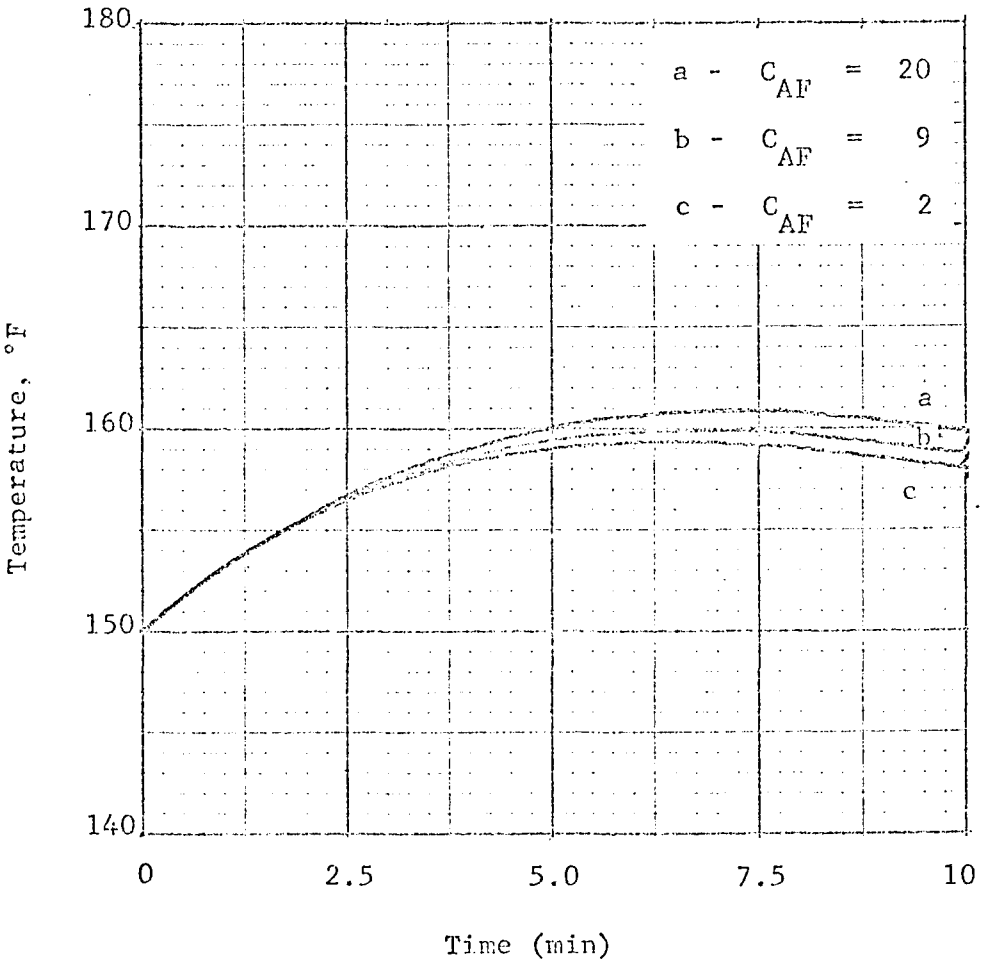


Figure V-22

Temperature Response for
Constant Disturbances in
Feed Concentration

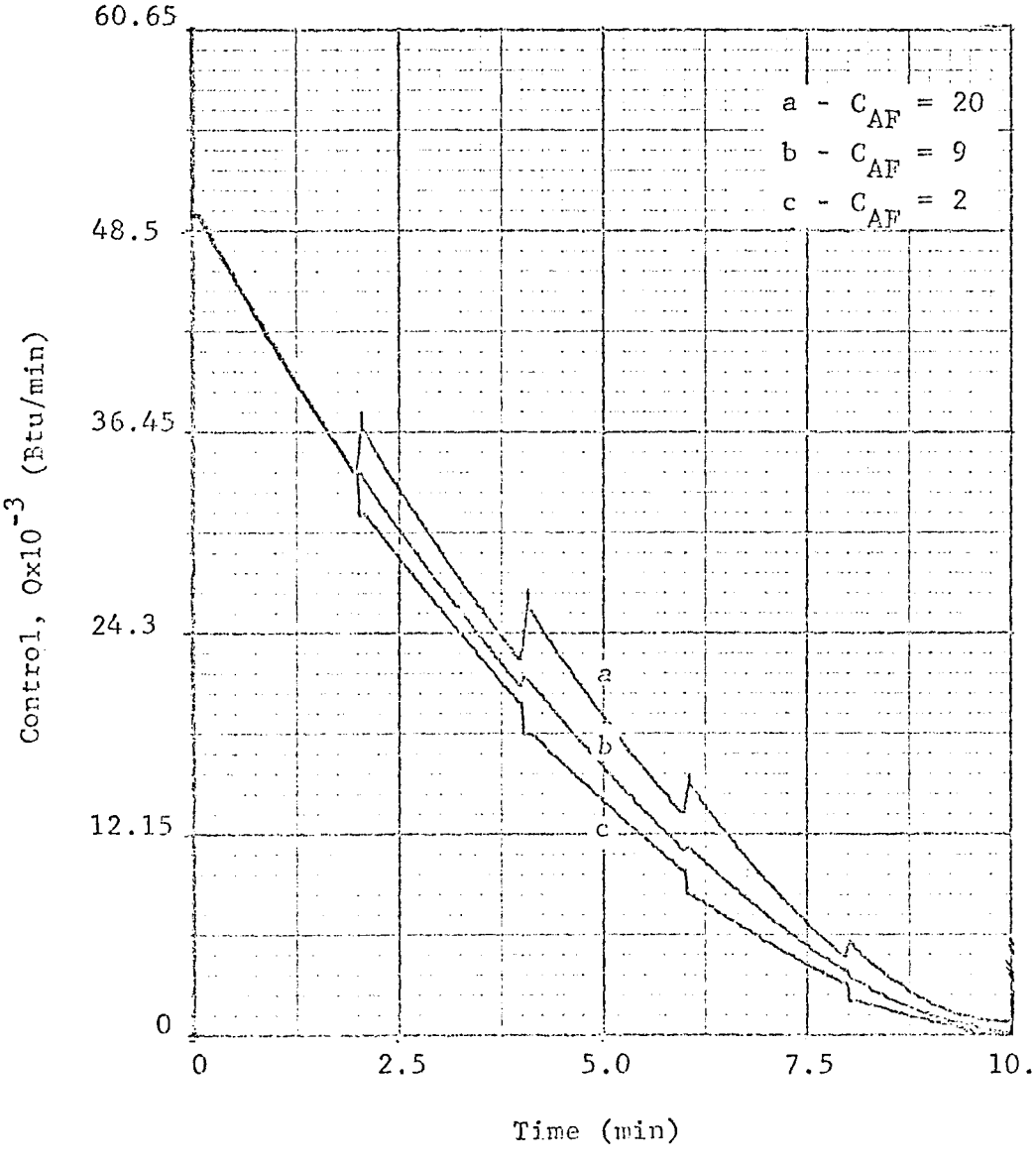


Figure V-23

Hybrid Control for Constant
Feed Concentration Disturbances

sampled, deviations from the precalculated temperature and concentration are detected and the control action is corrected as shown in Figure V-23. Note that less control action is needed for a feed concentration of 2 lb/ft^3. This is because the feed is entering in a highly reacted state and the additional Q is not needed. Figure V-23 is a dramatic illustration that the controller is working properly.

Figures V-24 through V-26 show the effect of changes in feed temperature. Figure V-24 is the concentration response for the two feed temperature disturbances (T_F = 90, 150). Note the increase in reaction rate (as shown by the lower concentrations) for the case with higher feed temperature. Figure V-25 is the effect on the reactor temperature. Figure V-26 is the hybrid control action for these disturbances. Note that much less correction is made than for feed concentration disturbances. This is because the control is a stronger function of concentration than temperature (note greater effect in Table V-2 of λ_1 and λ_2 on C_A than T) and is due to the fact that we are trying to minimize the integral of C_A^2 (not T^2). Figure V-26 shows controller is working properly. For the increase in feed temperature less heat transfer Q is needed and the proper correction is carried out. The opposite is also true for the decrease in feed temperature.

Conclusion

This example shows that the hybrid controller can be implemented for the feedback optimal control of complicated highly nonlinear systems.

It appears that the restricting factor in use of such a technique is the analog hardware required. Observe that in this example

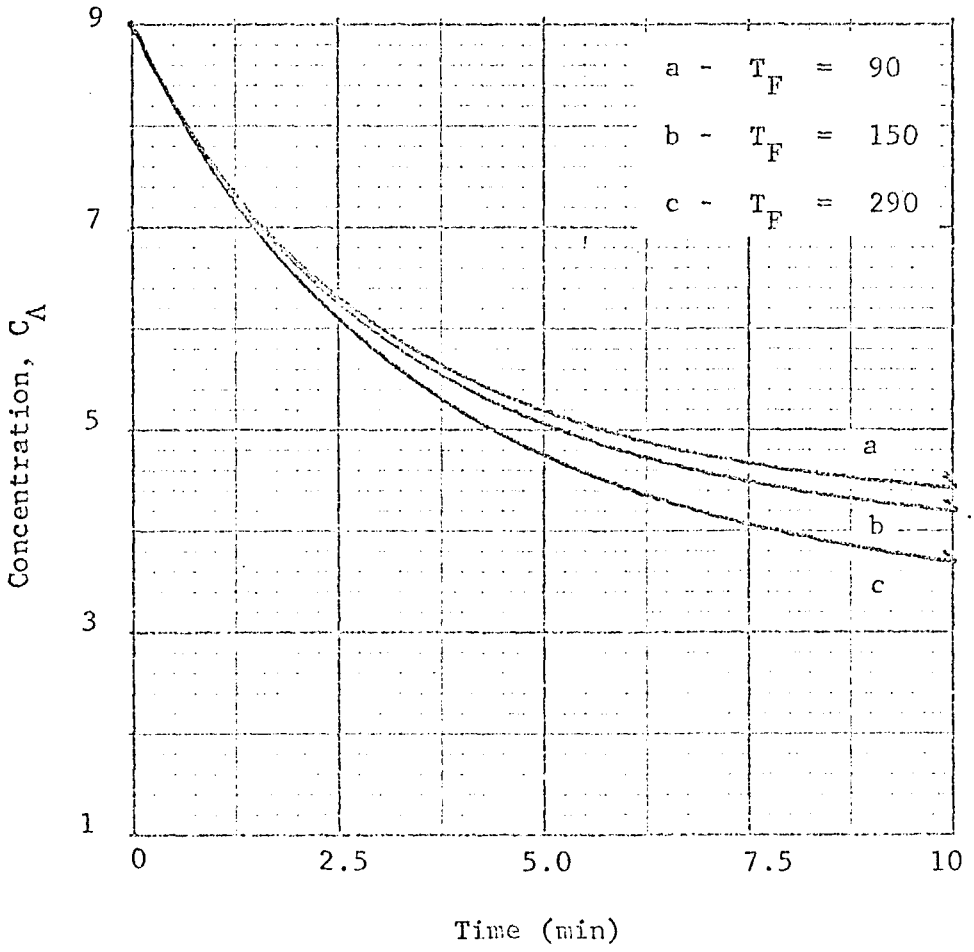


Figure V-24

Concentration Response for
Constant Disturbances in
Feed Temperature

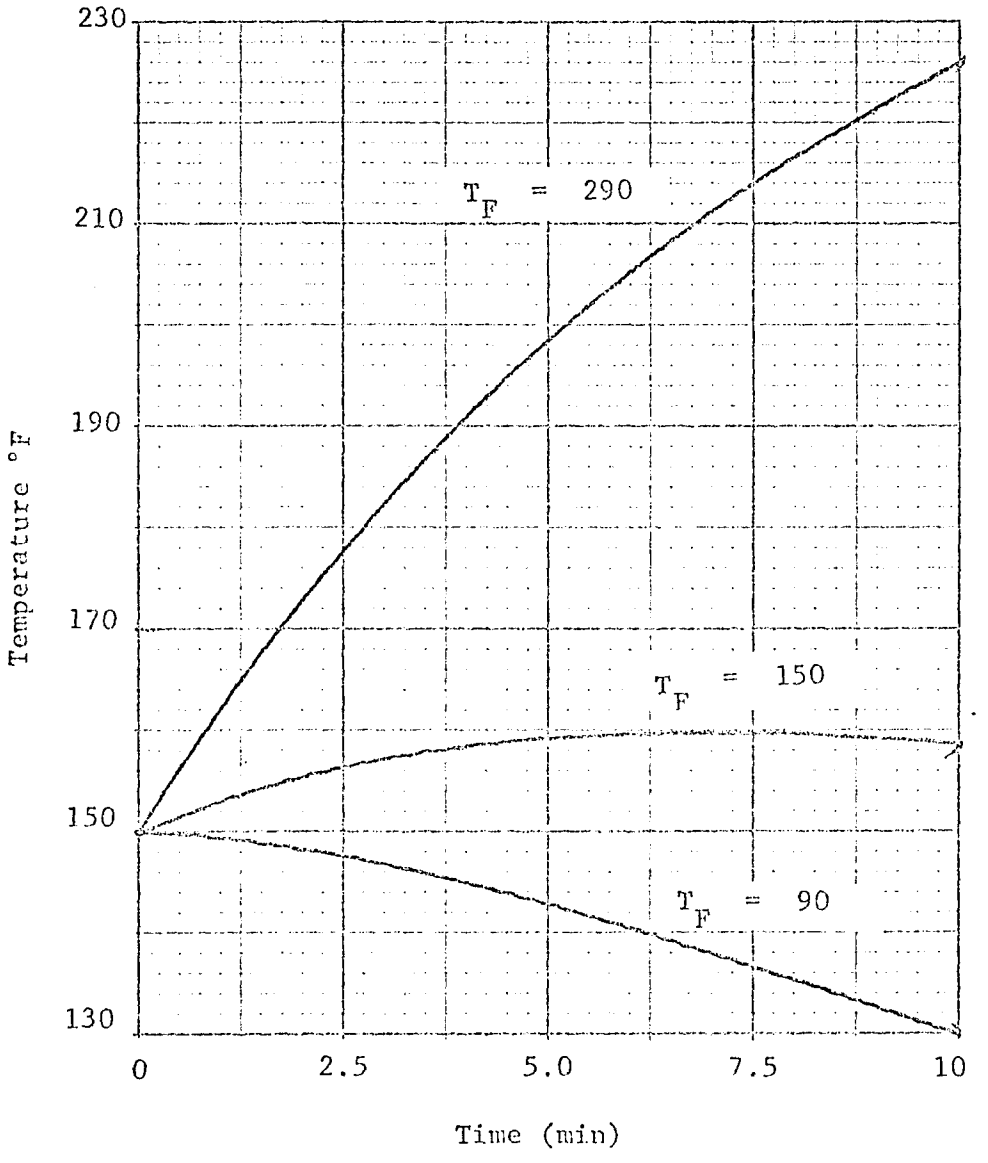


Figure V-25

Temperature Response for
Constant Disturbances in
Feed Temperature

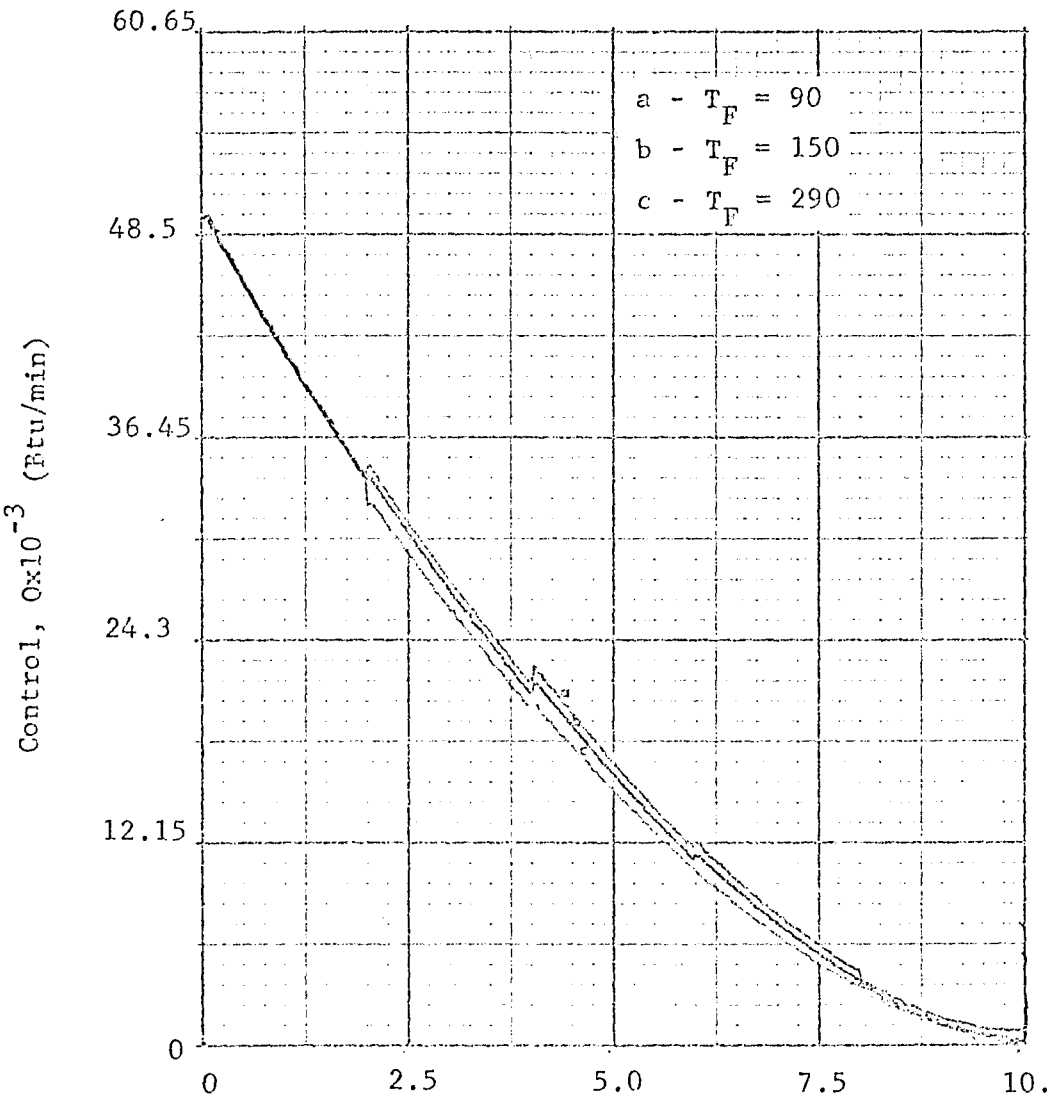


Figure V-26

Hybrid Control for Constant Feed Temperature Disturbances

the controller required 21 amplifiers of which 5 are integrators. Twelve nonlinear pieces of equipment (multipliers, dividers and squarers) were also needed.

Nomenclature

A - Parameter in Arrhenius temperature equation

ADC - Analog to Digital Converter

C_A - Concentration of reactant A

C_A^i - Concentration of A obtained on ith iteration

C_{AD} - Desired initial concentration of A

C_{Af} - Concentration of feed

C_p - Heat capacity of reactor contents

DAC - Digital to Analog Converter

H - Hamiltonian function

J - Performance criterion

Q - Heat transfer

SQ - Squarer

T - Absolute temperature

T_D - Desired initial temperature

V - Volume of reactor

W - Flow rate of feed to reactor

b - Constant term in performance criterion

f - Nonlinear function

g - Nonlinear function

k - Reaction rate constant defined by equation V-12

k_o - Frequency factor

t - Time

t_f - Final time

t_o - Initial time

t_s - Sampling time

$u(t)$ - Control function

$u^*(t)$ - Optimal control function

x - State variable

λ - Adjoint or costate variable

ρ - Density of reactor contents

ΔH - Heat of reaction

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CHAPTER VI

CONCLUSION

Approximate and short-cut methods were developed in this dissertation for the optimal control of nonlinear systems. It was shown that good approximations to the theoretical optimal can be obtained and that, in many cases, considerable savings in computations also result.

In Chapter II, graphical techniques were developed which allow the user to easily and rapidly obtain the optimal temperature or temperature profile for homogeneous, reversible, exothermic reactions.

In Chapter III, a direct finite difference method was developed and applied to a variety of linear and nonlinear optimal control problems. This reduced the solution of the optimal control problem to the solution of a set of algebraic equations. It was shown that this method gives good results and, in many cases, is simpler and more straightforward than conventional procedures.

Chapter IV consists of the use of a multidimensional search technique to determine approximate optimal feedback control algorithms for nonlinear systems. This method proved to give better results than does linearization and the application of optimal control theory.

In Chapter V, the problem of approximate optimal feedback

control of nonlinear systems was also considered. A theoretical approach was taken that resulted in a "hybrid controller". This controller was shown to be able to compensate for large disturbances.

APPENDIX A

COMPUTER PROGRAMS FOR CHAPTER II

```
C
C
C    PROGRAM USED FOR CALCULATING AND PLOTTING OF OPTIMAL ISOTHERMAL
C    TEMPERATURE FOR REVERSIBLE REACTIONS
C    PLOTTING SUBROUTINES ARE FOR CALCOMP PLOTTER
C
      DIMENSION A(1),GRD(1),GRD1(1)
      DIMENSION RLE(2,60)
      DIMENSION XP(700),YP(700),YPP(700)
      COMMON ALPH,B,X0,TEMPT,A41,AM1
      CALL PLOTS(RLE,5000)
      CALL PLOT (0.,0.,-3)
C  NCYC=NUMBER OF LOG CYCLES ON ABSISIA
      READ(5,1)NCYC
    1 FORMAT(I2)
C    READ IN INITIAL VALUE OF PARAMETERS
      READ(5,10)ALPH,B,AM1
   10 FORMAT(3F10.0)
C
C    B=DIMENSIONLESS PARAMETER
C    AM1=RATIO OF INITIAL CONCENTRATIONS
      K=1
      NPT=(NCYC*90)+1
      NP1=NPT+1
      NP2=NPT+2
      BSAVE=B
      XP(NP1)=BSAVE
      XP(NP2)=1.0
      YPP(NP1)=1.
      YPP(NP2)=.2
      YP(NP1)=.1
      YP(NP2)=.6
   19 X0=X1
   11 B1=B
      DO 3 I=1,6
```

```
      B=B1
      WRITE(6,12)ALPH,B,AMM
   12 FORMAT(1X,F,2,6)
      DO 4 J=1,NPT
C     SETTING LIMITS OF MAX AND MIN VALUES OF TEMP.
      XMAX=15.
      XMIN=0.
   20 TEST=XMAX+(B*(XMAX**ALPH))
      IF(TEST .LT.400.)GO TO 40
      XMAX=XMAX*.9
      GO TO 20
   40 CONTINUE
      SAV=XMAX
C
C     SUBROUTINE GOS IS THE GOLDEN SECTION SEARCH TECHNIQUE
C     USED TO MAXIMIZE CONVERSION
      CALL GOS(XMIN,XMAX,B,ERR,XOPT,COST)
C     B,ERR=ERROR TERMS
C     XOPT=RESULTING OPTIMAL DIMENSIONLESS TEMP.
C     COST=RESULTING MAX VALUE OF CONVERSION
C
C     TEST TO SEE IF OPTIMUM IS ON THE BOUNDRY
C     IF OPTIMUM IS ON BOUNDRY ADJUST CONSTRAINTS
      BTEST=ABS(SAV-XOPT)
      IF( BTEST .LT..3 )GO TO 50
      WRITE(6,501)
  501 FORMAT(1X,18HOPTIMUM ON BOUNDRY)
      XMAX=XMAX+1.5
      GO TO 6
  500 CONTINUE
      YP(J)=XOPT
      YPP(J)=COST
      XP(J)=T
C     PROVISION FOR EVEN SPACING OF PTS ON ABS.(LOG)FOLLOWS
      IF(J.LE.30)GO TO 70
```

```
      IF(J.LE.180)GO TO 71
      IF(J.LE.270)GO TO 72
      IF(J.LE.360)GO TO 73
      IF(J.LE.450)GO TO 74
      IF(J.LE.540)GO TO 75
      IF(J.LE.630)GO TO 76
   70 DX=DSAVE/10.
      GO TO 4
   71 DX=DSAVE
      GO TO 4
   72 DX=DSAVE*10.
      GO TO 4
   73 DX=DSAVE*100.
      GO TO 4
   74 DX=DSAVE*1000.
      GO TO 4
   75 DX=DSAVE*10000.
      GO TO 4
   76 DX=DSAVE*100000.
    4 X=X+DX
      WRITE(6,40)(XP(I),YP(I),YPP(I))
   40 FORMAT(1X,3F20.5)
C  DRAWING AXIS FOLLOWS
      IF(K-1)30,31,30
   31 CALL LOGAXIS(0.,0.,ARG,+1,5.,2).,YP(NP1),YP(NP2))
      CALL LOGAXIS(0.,0.,AR,-1,5.,0.,XP(NP1),XP(NP2))
      CALL PLOT(0.,5.,+3)
      CALL PLOT(5.,5.,+2)
      CALL PLOT(5.,0.,+2)
      CALL LOGAXIS( 5.,0.,AR,-1,5.,0.,XP(NP1),XP(NP2))
      CALL AXIS( 5.,0.,ARG1,+1,5.,2).,YPP(NP1),YPP(NP2))
      CALL PLOT(5.,5.,+3)
      CALL PLOT(10.,5.,+2)
      CALL PLOT(10.,0.,+2)
      K=2
```

```
   30 CONTINUE
      CALL PLOT(0.,0.,-3)
C     PLOT OPTIMAL TEMP. AND CONVERSION VS. PARAMETER B
      CALL LGLINE(XP,YP,NPT,1,0,0,0)
      CALL PLOT( 5.,0.,-3)
      CALL LGLINE(XP,YP2,NPT,1,0,0,-1)
      CALL PLOT(-5.,0.,-3)
    3 ALP=ALP+.5
      CALL PLOT(0.,0.,999)
      STOP
      END
C
C
      SUBROUTINE GOLD(XMIN,XMAX,E,ERR,XOPT,COST)
C
C*****GOLDEN SECTION SEARCH FOR 1 DIMENSIONAL MAXIMATION
C*****XMIN=MINIMUM VALUE OF INDEPENDENT VARIABLE
C*****XMAX=MAXIMUM VALUE OF INDEPENDENT VARIABLE
      J=0
      I=0
    5 X1=XMIN+.382*(XMAX-XMIN)
      CALL FNC(X1,COST1)
      J=J+1
      IF(J.GT.150)GO TO 100
      IF(I-1)6,7,7
    6 X2=XMIN+.618*(XMAX-XMIN)
      CALL FNC(X2,COST2)
      J=J+1
      IF(J.GT.150) TO 100
    7 ERR=ABS(XMAX-XMIN)
      IF(COST1-COST2)1,1,2
CASE WHERE COST1 IS GREATER
    2 XMAX=X2
      XP=X1
      COST=COST1
```

```
      I=1
      IF(F
     .LT. E)GO TO 10
      GO TO 5
CASE WHERE COST2 IS GREATER
    1 X=J
      XJ=.6
      COST1=COST2
      I=2
      IF(F
     .LT. E)GO TO 10
      GO TO 6
  100 WRITE(6,101)
  101 FORMAT(1X,'ADDRESS TERMINATED DO TO TOO MANY ITERATIONS')
   10 XOPT=X
      COST=COST1
      RETURN
      END
C
C
      SUBROUTINE PRO(T,COST)
C
C   SUBROUTINE PRO IS INTEGRATED RATE EQUATION
C   THIS SUBROUTINE IS THE INTEGRATED DIMINSIONLESS RATE EQUATION
C   NOTE ONLY THIS SUBROUTINE CHANGES FOR THE DIFFERENT REACTIONS
C   FIRST ORDER REV. REACTION SHOWN HERE
C
      COMMON AA,AB,AC,AD,AE,AF,AG
      DOUBLE PRECISION U,X,A1,B1,C1,D,CM,S0,BC2,B2,A2,C2,XK,ALPH,X0,B,AM
     1,D,C
      ALPH=AA
      B=AB
      A1=AC
      XJ=AC
      U=T
      X=0.
      D=U+(2*(J**ALPH))
```

```
      C=EXP(XMU(I))
      X(I,J)=(1./(1.+C))*(U(I,J)-(1.-U(I,J))*(1./(1.+C)))
    6 CONTINUE
      RETURN
      END
```

APPENDIX B

COMPUTER PROGRAMS FOR CHAPTER III

```
C
C
C    THIS PROGRAM CALCULATES THE OPTIMAL CONTROL FOR THE LINEARIZED
C    REACTOR BY BACKWARD INTEGRATION OF THE MATRIX RICCATI EQUATION
C
      DIMENSION A(2,2),B(2,2),AT(2,2),BT(2,2),RINV(2,2),Q(2,2),AK(2,2),P
     1ROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),T1(2,2),T2(2,2),C(5),ST
     1EP(5),SUM(2,2)
C
C    READ IN SYSTEM AND PERFORMANCE INDEX PARAMETERS
C    A=SYSTEM MATRIX
C    B=CONTROL MATRIX
C    RINV=INVERSE OF R MATRIX FOR P.I.
C    Q=Q MATRIX OF P.I.
C    TF=FINAL TIME
C    DT=DELTA TIME FOR NUMERICAL INTEGRATION
C
      READ(5,2)((A(I,J),J=1,2),I=1,2)
    2 FORMAT(2F10.0)
      READ(5,2)((B(I,J),J=1,2),I=1,2)
      READ(5,2)((RINV(I,J),J=1,2),I=1,2)
      READ(5,2)((AK(I,J),J=1,2),I=1,2)
      WRITE(6,3)((A(I,J),J=1,2),I=1,2)
      WRITE(6,3)((B(I,J),J=1,2),I=1,2)
      WRITE(6,3)((AK(I,J),J=1,2),I=1,2)
    3 FORMAT(2F10.2)
      READ(5,2)((Q(I,J),J=1,2),I=1,2)
      READ(5,10)TF,DT
   10 FORMAT(2F10.0)
      CALL PROC
      STOP
      END
C
C
      SUBROUTINE PROC
```

```
C
C    THIS SUBROUTINE SOLVES THE RICCATI EQU. AND GENERATES THE REACTOR
C    RESPONCE
       COMMON A,B,RINV,Q,AK ,SUM,TF,DT
       DIMENSION A(2,2),B(2,2),AT(2,2),BT(2,2),RINV(2,2),Q(2,2),AK(2,2),P
      1R0D1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),T1(2,2),T2(2,2),SUM(2,2
      1),C(5)
       DIMENSION S1(500),S2(500),S3(500)
       DIMENSION RINVN(2,2)
       TIME=0.
       IT=TF/DT+1.5
       IN=0
C    CALCULATE TRANSPOSE OF A AND B MATRIX
       DO 10 I=1,2
       DO 10 J=1,2
       AT(I,J)=A(J,I)
    10 BT(I,J)=B(J,I)
       N=2
       M=2
       NP=2
C
C    SUBROUTINE PROD4 FORMS THE PRODUCT OF TWO MATRICES
C
   100 CALL PROD4(AK,A,PROD1,N,M,NP)
       DO 50 I=1,2
       DO 50 J=1,2
    50 T1(I,J)=PROD1(I,J)
       CALL PROD4(AT,AK,PROD1,N,M,NP)
       DO 51 J=1,2
       DO 51 I=1,2
    51 T2(I,J)=PROD1(I,J)
       CALL PROD4(AK,B,PROD1,N,M,NP)
       CALL PROD4(PROD1,RINV,PROD2,N,M,NP)
       CALL PROD4(PROD2,BT,PROD3,N,M,NP)
       CALL PROD4(PROD3,AK,PROD4,N,M,NP)
```

```
      DO 60 I=1,2
      DO 60 J=1,2
C
C    SUM(I,J) IS THE RICCATI EQU.
C
   60 SUM(I,J)=-T1(I,J)-TP(I,J)+PROD4(I,J)-Q(I,J)
      DO 61 I=1,2
      DO 61 J=1,2
C    BACKWARD INTEGRATION
   61 AK(I,J)=AK(I,J)-SUM(I,J)*DT
      TIME=TIME-TIME
      WRITE(6,71)TIME
   71 FORMAT(1X,'TIME=',F10.4)
      TIME=TIME+DT
      WRITE(6,70)((AK(I,J),J=1,2),I=1,2)
   70 FORMAT(1X,                    2E15.5)
      JJ=IT-IN
C    RESULTS STORED IN S1,S2,S3 AND USED TO GENERATE THE OPTIMAL CONTROL
      S1(JJ)=AK(1,1)
      S2(JJ)=AK(2,1)
      S3(JJ)=AK(2,2)
      IN=IN+1
      IF(TIME.LT.TF)GO TO 100
C
      X1=20.
      X2=.5
C
      DO 20 I=1,2
      DO 20 J=1,2
   20 RINV(I,J)=-RINV(I,J)
      J=0
   22 J=J+1
      IF(J.NE.1)GO TO 24
      PROD3(1,1)=0.
      PROD3(2,1)=0.
```

```
      PROD3(1,2)=0.
      PROD3(2,2)=0.
   35 CONTINUE
      F1=A(1,1)*X1+A(1,2)*X2+PROD3(1,1)*X1+PROD3(1,2)*X2
      F2=A(2,1)*X1+A(2,2)*X2+PROD3(2,1)*X1+PROD3(2,2)*X2
C
C    SYSTEM RESPONSE IS GENERATED BY FORWARD INTEGRATION OF SYSTEM EQUS.
C    WITH CONTROL FROM RICCATI SOLUTION
C
      X1=X1+F1*DT
      X2=X2+F2*DT
      AK(1,1)=S1(J)
      AK(2,1)=S2(J)
      AK(1,2)=S3(J)
      AK(2,2)=S4(J)
      WRITE(6,70)((AK(I,L),L=1,2),I=1,2)
      CALL PROD1(AINV,RT,PROD1,N,NP,M)
      CALL PROD1(PROD1,AK,PROD2,N,NP,M)
      U1=PROD2(1,1)*X1+PROD2(1,2)*X2
      U2=PROD2(2,1)*X1+PROD2(2,2)*X2
      CALL PROD1(B,PROD2,PROD3,N,NP,M)
      WRITE(6,21)J,X1,X2,U1,U2
   21 FORMAT(1X,I3,4E20.5)
      IF(J.LT.IT)GO TO 22
      RETURN
      END
C
C
      SUBROUTINE PROD1(AA,BB,PROD,N,M,NP)
C
C    SUBROUTINE TO MULTIPLY MATRIX AA TIMES BB
C
C    N=ROWS IN AA
C    M=COLUMNS IN AA AND ROWS IN BB
C    NP=COLUMNS IN BB
```

```
C     NOTE RESULT IS N BY NP
      DIMENSION AA(2,2),BB(2,2),PROD(2,2)
      DO 1 I=1,N
      DO 1 J=1,NP
      PROD(I,J)=0.
      DO 1 L=1,M
    1 PROD(I,J)=PROD(I,J)+AA(I,L)*BB(L,J)
      RETURN
      END
```

```
C
C
C     THIS PROGRAM DETERMINES THE OPTIMAL CONTROL FOR THE LINEARIZED
C     STIRRED TANK REACTOR USING THE DIRECT FINITE DIFFERENCE METHOD
C     NEWTON'S METHOD IS USED TO SOLVE THE RESULTING EQUATIONS
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,NP1,N2P1,N3P2,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200),SAVE(1200)
  500 READ(5,1)N,DT,X10,X20
C     N=NUMBER OF INCREMENTS
C     DT=DELTA TIME
    1 FORMAT(I3,3F10.0)
      WRITE(6,501)N,DT
  501 FORMAT(1X,'INCREMENTS=',I3,/1X,'DT=',F10.5)
      WRITE(6,505)X10,X20
C     X10=INITIAL VALUE OF TEMPERATURE
C     X20=INITIAL VALUE OF CONCENTRATION
  505 FORMAT(1X,'INITIAL CONDITIONS=',2F20.5)
C     DEFINITION PARAMETERS FOR SETTING UP ALGEBRAIC EQUS.
      K=1
      KKK=1
      NP1=N+1
      N2=N*2
      N2P1=N2+1
      N3=N*3
      N3P1=N3+1
      N4=N*4
      N4P1=N4+1
      N5=N*5
      N5P1=N5+1
      N6=N*6
C
C     SYSTEM PARAMETERS FOLLOW
C     ELEMENTS OF A MATRIX
```

```
      A11=.941
      A12=-.1
      A22=-.907
      A21=-.001
C     ELEMENTS OF B MATRIX
      B11=.001
      B12=-.136
      B22=.001
C
C     P.I. PARAMETERS FOLLOW
C
      R11=.01
      R22=1.
      Q11=10.
      Q22=100.
C
C     INITIALIZING VARIABLES
C
      DO 20 I=1,N6
   20 X(I)=1.
      DO 30 I=1,N3
   30 SAVE(I)=0.
C
C     WEIGHTING FACTOR FOR NEWTONS METHOD
C
      W=1.
C
C     EQUATIONS ARE NUMBERED AS FOLLOWS SO THAT THE COEFFICIENT OF X(N)
C     IN F(N) IS AS LARGE IN ABSOLUTE VALUE AS ANY OF THE REMAINING COEFFS
C     X(1-N)=A1
C     X(N+1-2N)=A2
C     X(2N+1-3N)=LAMBDA1
C     X(3N+1-4N)=LAMBDA2
C     X(4N+1-5N)=Y1
C     X(5N+1-6N)=Y2
```

```
C
C
  100 DO 8 I=1,N
C
C   SUBROUTINE 01 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT LAMBDA1
C
      CALL 01
C   ALGORITHM FOR NEWTON'S METHOD--- F(I) AND D(I) ARE GENERATED  IN
C   THE 6 SUBROUTINES BASED ON PRESENT VALUES OF X(I)
    2 X(I)=X(I)-W*(F(I)/D(I))
      K=K+1
      DO 3 I=NP1,N2
C
C   SUBROUTINE 02 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT LAMBDA2
C
      CALL 02
    3 X(I)=X(I)-W*(F(I)/D(I))
      DO 4 I=N2P1,N3
C
C   SUBROUTINE 03 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT TEMP
C
      CALL 03
    4 X(I)=X(I)-W*(F(I)/D(I))
      DO 5 I=N3P1,N4
C
C   SUBROUTINE 04 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT CON.
C
      CALL 04
    5 X(I)=X(I)-W*(F(I)/D(I))
      DO 6 I=N4P1,N5
C
C   SUBROUTINE 05 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT HEAT TRAN.
C
      CALL 05
    6 X(I)=X(I)-W*(F(I)/D(I))
```

```
      DO 7 I=1,N6
C
C   SUBROUTINE G6 GENERATES EQUATIONS RESULTING FROM PARTIALS WRT FLOW
C
      CALL G6
    7 X(I)=X(I)-W*(F(I)/D(I))
      IF(KKK.GT.2000)GO TO 42
      TEST=0.
      DO 20 I=1,N6
   20 TEST=TEST+ABS(SAVE(I)-X(I))
C   TEST FOR CONVERGENCE BY COMPARING CHANGE IN VALUE OF VARIABLES
C   FROM ONE ITERATION TO THE NEXT
      IF(TEST.LT..01 )GO TO 202
      KKK=KKK+1
      IF(KKK.EQ.100)GO TO 300
      GO TO 302
  300 WRITE(6,301)TEST
  301 FORMAT(1X,'TEST=',F20.5)
      KKK=0
  302 CONTINUE
      DO 90 I=1,N6
C   STORE PRESENT VALUE OF UNKNOWNS X(I) FOR CONVERGENCE TEST
   90 SAVE(I)=X(I)
      GO TO 100
  202 WRITE(6,41)K
   41 FORMAT(1X,'NUMBER OF ITERATIONS NEEDED=',I5)
      GO TO 24
   42 WRITE(6,43)
   43 FORMAT(1X,'SYS DRT CONVERGE AFTER 2000 ITERATIONS!')
   24 CONTINUE
      WRITE(6,210)(I,X(I),F(I),I=1,N6)
  210 FORMAT(10X,I5,2F20.5)
      GO TO 900
      STOP
      END
```

```
C
C
      SUBROUTINE G1
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO LAMBDA1
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N6,NP1,N2P1,N3P2,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
C     D(I) IS DENOMINATOR TERM FOR NEWTON'S METHOD
      D(I)=1.
      IF(I.GT.(N-1))GO TO 1
      F(I)=X(I)-X(I-1)-A11*X(I-1)*DT-A12*X(I+N-1)*DT-B11*X(I+N4)*DT-B12*
     1X(N4+I)*DT
      GO TO 2
    1 F(I)=X(I)-X10*(1.+A11*DT)-A12*X20*DT-B11*X(N4+I)*DT-B12*X(I+N5)*DT
    2 RETURN
      END
C
C
      SUBROUTINE G2
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO LAMBDA2
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N6,NP1,N2P1,N3P2,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
      D(I)=1.
      IF(I.GT.(N+NP1))GO TO 1
      F(I)=X(I)-X(I-1)-A21*X(I-NP1)*DT-A22*X(I-1)*DT-B22*X(I+N4)*DT
      GO TO 2
    1 F(I)=X(I)-X20*(1.+A22*DT)-A21*X10*DT-B22*X(I+N4)*DT
    2 RETURN
```

```
      END
C
C
      SUBROUTINE G2
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO X1 (TEMPERATURE)
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N1P1,N2P1,N3P1,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
      D(I)=1.
      IF(I.EQ.N3) GO TO 1
      F(I)=2.*Q11*DT*X(I-N2)-A11*DT*X(I+1)+X(I)-A21*DT*X(I+N+1)-X(I+1)
      GO TO 2
    1 F(I)=X(I)
    2 RETURN
      END
C
C
      SUBROUTINE G4
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO X2 (CONCENTRATION)
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N1P1,N2P1,N3P1,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
      D(I)=1.
      IF(I.EQ.N4) GO TO 1
      F(I)=2.*Q22*DT*X(I-N2)-A22*DT*X(I+1)+X(I)-A12*DT*X(I-N+1)-X(I+1)
      GO TO 2
    1 F(I)=X(I)
    2 RETURN
      END
```

```
C
C
      SUBROUTINE G5
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO U1 (HEAT TRANSFER)
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N6,NP1,N2P1,N3P1,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
      F(I)=2.*A11*X(I)-X(I-N2)*A11
      D(I)=2.*B11
    2 RETURN
      END
C
C
      SUBROUTINE G6
C
C     THIS SUBROUTINE GENERATES THE N EQUATIONS RESULTING FROM PARTIALS
C     WITH RESPECT TO U2 (FLOW RATE)
C
      COMMON I,N,X,F,D,DT,A11,A21,A22,B11,B12,B22,R11,R22,X10,X20,Q11,Q2
     12,N2,N3,N4,N5,N6,NP1,N2P1,N3P1,N4P1,N5P1,A12
      DIMENSION F(1200),X(1200),D(1200)
      F(I)=2.*B22*X(I)-B12*X(I-N3)-B22*X(I-N2)
      D(I)=2.*B22
      RETURN
      END
```

APPENDIX C

COMPUTER PROGRAMS FOR CHAPTER IV

```
C
C
C     THIS IS THE MAIN PROGRAM FOR STUDY IN CHAPTER 4
C     PROGRAM USED TO DETERMINE CONTROLLER BASED ON LINEARIZATION
C     AND BASED ON SEARCH OF THE NON-LINEAR SYSTEM --- ALSO USED TO
C     CALCULATE AND PLOT RESPONSES
C
      COMMON VOL,DEN,DELH,CP,AKS,US,CS,DT,FTIME,X10,X20,Z,AKO,TFS,CFS,TO
     2UTS,COUTS,A,B,P,F,RINV,RK,N,NP,M,AT,BT,PROD2,JOPT,XP,Y1,Y2,Y3,Y4,N
     3PT
      DIMENSION RINV(2,2),P(2,2),A(2,2),AT(2,2),B(2,2),BT(2,2),RK(2,2),A
     1A(2,2),F(2,2),PROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),PROD5(2
     2,2),PROD6(2,2),SUM(2,2),P(2,2),RINVM(2,2),C(10),STEP(10),XP(500),Y
     31(500),Y2(500),Y3(500),Y4(500),BUF(5000)
      N=2
      NP=2
      M=2
C     NPP=NO.PARAMETERS TO BE DETERMINED BY SEARCH
C     NPASS=NO.PASSES IN PATTERN SEARCH
C     STEP=INITIAL STEP SIZE FOR PATTERN SEARCH
      READ(5,40)NPP,NPASS,IP
   40 FORMAT(3I2)
      READ(5,41)(STEP(I),I=1,NPP)
   41 FORMAT(F10.0)
C     READING IN REACTOR PARAMETERS
      READ(5,1)VOL,DEN,CP,DELH,Z,AKO
    1 FORMAT(6F10.0)
      WRITE(6,30)
   30 FORMAT(1H1,3HVOL,12X,3HDEN,12X,2HCP,12X,4HDELH,13X,1HZ,13X,3HAKO)
      WRITE(6,10)VOL,DEN,CP,DELH,Z,AKO
   10 FORMAT(1X,6E15.3)
C     READING IN STEADY STATE VALUES OF FEED AND SETPOINTS OF OUTPUTS
      READ(5,2)TFS,CFS,TOUTS,COUTS
    2 FORMAT(4F10.0)
      WRITE(6,31)
```

```
   31 FORMAT(//,20X,'STEADY STATE FEED AND OUTPUT (SET PT.) CONDITIONS',//
     1 20X,'SET PT.',15X,'FEED CON.',12X,'SS P.TEMP',12X,'SS P.CON.')
       WRITE(6,11)FES,SFS,TOUTS,COUTS
   11 FORMAT(3X,4E25.5)
C    READING IN STEP SIZE AND FINAL TIME
       READ(5,3)DT,FTIME
    3 FORMAT(2F10.0)
       WRITE(6,14)DT,FTIME
   14 FORMAT(3X,F10.5)
C    READING IN PARAMETERS THAT SPECIFY PERFORMANCE INDEX
       READ(5,21)((Q(I,J),J=1,2),I=1,2)
   21 FORMAT(4F10.0)
       WRITE(6,32)
   32 FORMAT(2X,//'Q MATRIX')
       WRITE(6,33)((Q(I,J),J=1,2),I=1,2)
   33 FORMAT(1X,2E15.8)
       READ(5,23)((RINV(I,J),J=1,2),I=1,2)
   23 FORMAT(4F10.0)
       READ(5,101)((C(I,J),J=1,2),I=1,2)
  101 FORMAT(4F10.0)
       WRITE(6,34)
   34 FORMAT(1X,//'S*R MATRIX')
       WRITE(6,35)((S(I,J),J=1,2),I=1,2)
   35 FORMAT(1X,2E15.8)
C    READING IN INITIAL CONDITIONS ON STATE VARIABLES, TEMP AND CON.
  100 READ(5,4)X10,X20
    4 FORMAT(2F10.0)
       WRITE(6,36)
   36 FORMAT(1X,'INITIAL CONDITIONS')
       WRITE(6,12)X10,X20
   12 FORMAT(1X,F10.5)
       WRITE(6,20)((RINV(I,J),J=1,2),I=1,2)
   20 FORMAT(2X,2E15.4)
       CALL PLOT(0.,0.,-3)
       NPT=FTIME/DT+.5
```

```
NP1=NP1+1
NP2=NP1+2
XP(NP1)=0.
XP(NP2)=20.
Y1(NP1)=0.
Y1(NP2)=6.
Y2(NP1)=0.
Y2(NP2)=.12
Y3(NP1)=-200.
Y3(NP2)=40.
Y4(NP1)=0.
Y4(NP2)=8.
CALL AXIS(0.,0.,4HTIME,-4,5.,0.,XP(NP1),XP(NP2))
CALL AXIS(0.,0.,11HTEMPERATURE,+11,5.,90.,Y1(NP1),Y1(NP2))
CALL PLOT(0.,5.,+3)
CALL PLOT(5.,5.,+2)
CALL PLOT(5.,0.,+2)
CALL AXIS(2.,0.,4HTIME,-4,5.,0.,XP(NP1),XP(NP2))
CALL AXIS(2.,0.,13HCONCENTRATION,+13,5.,90.,Y2(NP1),Y2(NP2))
CALL PLOT(6.,5.,+3)
CALL PLOT(11.,5.,+2)
CALL PLOT(11.,0.,+2)
XP(NP2)=14.
CALL AXIS(14.,0.,4HTIME,-4,5.,0.,XP(NP1),XP(NP2))
CALL AXIS(14.,0.,1H3,+1,5.,90.,Y3(NP1),Y3(NP2))
CALL PLOT(14.,5.,+3)
CALL PLOT(21.,5.,+2)
CALL PLOT(21.,0.,+2)
CALL AXIS(24.,0.,4HTIME,-4,5.,0.,XP(NP1),XP(NP2))
CALL AXIS(24.,0.,1H4,+1,5.,90.,Y4(NP1),Y4(NP2))
CALL PLOT(24.,5.,+3)
CALL PLOT(29.,5.,+2)
CALL PLOT(29.,0.,+2)
XP(NP2)=30.
CALL STOPIT
```

```
      CALL AIC
      CALL SCANN
C
C     INITIAL GUESSES FOR PARAMETERS,C(I), ARE OBTAINED FROM CONTROLLER
C     OBTAINED BY LINEARIZATION
      C(1)=PARCOR(1,1)
      C(2)=PARCOR(1,2)
      C(3)=PARCOR(2,1)
      C(4)=PARCOR(2,2)
      JOPT=0
C
C     NOTE PATTERN SEARCH IS NOT LISTED *** PROGRAM IS REFERENCED IN
C     CHAPTER 4 AND MAY BE OBTAINED FROM IBM SHARE LIBRARY
C
      CALL PATERN(NPP,C,STEP,NPASS,IB,COST)
C
C     WHEN JOPT=1 SUBROUTINE PROC ONLY USED TO GENERATE RESPONCE
      JOPT=1
      CALL PROC(C,COST)
      CALL PLOT(0.,0.,999)
      STOP
      END
C
C
      SUBROUTINE AIC
C
C***THIS SUBROUTINE FORMULATES THE MATRIX RICCATI EQU. AND PREFORMS
C***FIRST ORDER BACKWARD INTEGRATION TO OBTAIN STEADY STATE SOLUTION
C
      COMMON NN,LEN,DELM,CP,AMS,IS,OS,DT,FTIME,X10,X20,Z,AKO,TFS,CFS,TS
     1UTS,COUTS,A,B,Q,R,RINV,SX,N,NP,M,AT,BT,PRODR,JOPT
      DIMENSION RINV(2,2),Q(2,2),A(2,2),AT(2,2),B(2,2),BT(2,2),RK(2,2),A
     1A(2,2),PM(2,2),PROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),PROD5(2
     2,2),PROD6(2,2),SUM(2,2),R(2,2),PRODR(2,2)
      IT=1.
```

```
C***SETTING BOUNDARY CONDITIONS AT FINAL TIME=0
      DO 1 I=1,P
      DO 1 J=1,P
    1 RK(I,J)=0.
  100 CONTINUE
      IT=IT+1
      CALL PROD1(RK, A,PROD1,N,NP,M)
      CALL PROD1(AT,RK,PROD2,N,NP,M)
      CALL PROD4(RK, M,PROD3,N,NP,M)
      CALL PROD1(PROD3,INV,PROD4,N,NP,M)
      CALL PROD1(PROD4,MT,PROD5,N,NP,M)
      CALL PROD1(PROD5,RK,PROD6,N,NP,M)
C   SUMMING MATRICES TO FORM SAC+ FOR.
      DO 7 I=1,P
      DO 7 J=1,P
C***SUM IS THE INTEGRATIVE MATRIX
    7 SUM(I,J)=-PROD1(I,J)-PROD2(I,J)+PROD6(I,J)-Q(I,J)
      DO 3 I=1,P
      DO 3 J=1,P
    3 RK(I,J)=RK(I,J)-SUM(I,J)*DT
C***INTEGRATION PROCEEDS UNTIL STEADY STATE IS REACHED
      TEST=ABS(SUM(1,1))+ABS(SUM(1,2))+ABS(SUM(2,1))+ABS(SUM(2,2))
      IF(IT.GT.1000.)GO TO 12
      IF(TEST.GT..1)GO TO 100
      GO TO 15
   12 WRITE(6,13)
   13 FORMAT(1X,//46HSTEADY STATE NOT REACHED AFTER 1000 ITERATIONS)
      WRITE(6,14)TEST
   14 FORMAT(1X,5HTEST=,F10.6)
   15 WRITE(6,10)((SUM(I,J),J=1,2),I=1,2)
   10 FORMAT(1X,2F15.4)
      WRITE(6,30)
   30 FORMAT(5X,23HRICCATI SOLUTION MATRIX)
      WRITE(6,11)((RK(I,J),J=1,2),I=1,2)
   11 FORMAT(1X,2F15.4)
```

```
      RETURN
      END
C
C
      SUBROUTINE STSTAT
C
C***THIS SUBROUTINE CALCULATES THE STEADY STATE VALUES OF OTHER VARIABLES
C***GIVEN THE SETPOINTS OF CONTROLLED VARIABLE AND FEED STEADY STATES
C***IT IS ALSO USED TO CALCULATE THE LINEARIZED A & B MATRICES
      COMMON VOL,DEN,DELH,CP,AKO,AS,BS,QS,QT,ETIME,X10,X20,Z,AKO,TFS,CFS,TO
     ZUTS,CBUTS,A,B,C,R,RINV,KK,N,NP,M,AT,BT,PROD2,JOPT
      DIMENSION RINV(2,2),R(2,2),A(2,2),AT(2,2),B(2,2),BT(2,2),RK(2,2),A
     1A(2,2),P(2,2),PROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),PROD5(2
     2,2),PROD6(2,2),SUM(2,2),P(2,2)
CALCULATION OF STEADY STATE VALUES OF OTHER VARIABLES
      AKS=AKO*(EXP(-Z/(TOUTS+460.)))
C   FROM STEADY STATE M.B. CALCULATE FEED FLOW
      FS=(AKS*(CBUTS**2)*VOL*DEN)/(CFS-CBUTS)
C   FROM STEADY STATE E.B. CALCULATE HEAT REQ.---NOTE NEG. Q IS HEAT REM
      QS=((FS+AKS*(CBUTS**2)*VOL)-(FS*CP*(TFS-TBUTS))
      WRITE(6,14)
   14 FORMAT(1X,//1HKS,9X,9HRATE CONSTANT,3X,18HS.S. REACTANT FLOW,3X,14HS
     1.S. HEAT DUTY)
      WRITE(6,13)AKS,FS,QS
   13 FORMAT(1X,3F20.6//)
      ABUTS=CBUTS+460.
C   CALCULATE STEADY STATE A MATRIX
      A(1,1)=-(FS/(VOL*DEN))-((2*DELH*AKS*(CBUTS**2))/(DEN*CP*(ABUTS**2)
     3))
      A(1,2)=-(2.*DELH*AKS*CBUTS )/(DEN*CP)
      A(2,1)=-(2*AKS*(CBUTS **2))/(ABUTS**2)
      A(2,2)=-(FS/(VOL*DEN))-(2.*AKS*CBUTS)
      WRITE(6,20)
   20 FORMAT(1X,27HLINEARIZED FORM OF A MATRIX)
      WRITE(6,15)((A(I,J),J=1,2),I=1,2)
```

```
   15 FORMAT(/5X,2F15.3)
C    CALCULATION OF B MATRIX
      B(1,1)=1./(2.*WL**2*CP)
      B(1,2)=(TFS-TOUTS)/(VOL*DEN)
      B(2,1)=0.
      B(2,2)=(CFS-COUTS)/(VOL*DEN)
      WRITE(6,21)
   21 FORMAT(//,5X,'LINEARIZED FORM OF B MATRIX')
      WRITE(6,11)((B(I,J),J=1,2),I=1,2)
   16 FORMAT(/,5X,2F15.3)
      DO 5 I=1,2
      DO 5 J=1,2
      AT(I,J)=A(J,I)
    5 BT(I,J)=B(J,I)
      RETURN
      END
C
C
      SUBROUTINE RICSOL
C
C***THIS SUBROUTINE IS USED TO GENERATE THE OPEN AND CLOSED LOOP
C***RESPONCE FOR THE LINEAR SYSTEM***COST IS EVALUATED
C***RICATTI CONTROLLER IS USED ON NONLINEAR SYSTEM
C
      COMMON /BLK/LEN,DELH,CP,AKC,IS,OS,DT,ETIME,X10,X20,Z,AKO,TFS,CFS,TO
     &UTS,COUTS,A,P,D,B,RINV,RK,N,NP,N,AT,BT,PROD2,JOPT
      DIMENSION RINV(2,2),D(2,2),A(2,2),AT(2,2),B(2,2),BT(2,2),RK(2,2),A
     1A(2,2),P(2,2),PROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),PROD5(2
     2,2),PROD6(2,2),SUM(2,2),X(2,2),XINVN(2,2)
C***NOTE D REPRESENTS NORMAL B MATRIX IN PERFORMANCE INDEX
      TIME=0.
      ATIME=0.
      DO 19 I=1,2
      DO 19 J=1,2
   19 RINVN(I,J)=-RINV(I,J)
```

```
      CALL PRODCT(A,INV,T,PROD1,N,NP,M)
      CALL PRODCT(B,PROD1,K,PROD2,N,MP,M)
      WRITE(6,50)((PROD2(I,J),J=1,2),I=1,2)
   50 FORMAT(1X,2F12.3)
      X1S=THETS
      X2S=OMETS
C     MANIPULATED VARIABLES ARE 0 FOR OPEN LOOP CASE
      Q=0.
      W=0.
C     OTHER NORMALIZED VARIABLES ARE 0 IF. STEADY STATE
      TF=0.
      CF=0.
      K=(RTIME/DT)+.5
      AITSP=0.
      AIT=0.
      X1=X10-X1S
      X2=X20-X2S
      X1OPEN=X1
      X2OPEN=X2
      FCOPEN=.5/(VOL*DEN)
C     NOTE THAT X1 AND X2 ARE TRANSFORMED VARIABLES SO THAT STEADY STATE
C     IS AT ORIGIN
      WRITE(6,30)
   30 FORMAT(5X,//64H OPEN LOOP LINEAR RESPONSE (OPEN & CLOSED LOOP) WITH RICAT
     1TI CONTROLLER)
      WRITE(6,31)
   31 FORMAT(2X,4HK=1,1X,2HX2,13X,4HX10P,10X,4HX20P,10X,1HQ,10X,1HW)
      DO1 I=1,K
      FACTOR=(I+.5)/(VOL*DEN)
      AKOPEN=AK*(EXP(-Z/(X10PEN+.67.)))
      AK=AKO*(EXP(-Z/(X1+.60.)))
      F1OPEN=FCOPEN*(TFS-(1.0PEN-X1S)+((QS)/(VOL*DEN*CP))-((DELH*(AK0PEN+
     1AKS)*((X2OPEN+X2S)**2))/(DEN*CP))
      F2OPEN=FCOPEN*(CFS-(X2OPEN-X2S)-(AK0PEN+AKS)*((X2OPEN+X2S)**2)
      F1=FACTOR*(TFSTFS-X1-X1S)+((Q+QS)/(VOL*DEN*CP))-((DELH*(AK+AKS)*((
```

```
     1X2+X2S)**2))/(DEN*DT)
      F1=FACTOR*(CF+CFS-X2-X2S)-(AK+AKS)*((X2+X2S)**2)
      ATIME=ATIME+DT
      TIME=TIME+DT
      X1=X1+(F1*DT)
      X2=X2+(F2*DT)
      X1DEN=X1DEN+(F1DEN*DT)
      X2DEN=X2DEN+(F2DEN*DT)
      U1=R1SD*(1,1)*X1+R1SD(1,2)*X2
      U2=R1SD(2,1)*X1+R1SD(2,2)*X2
      U=U1
      W=U2
      IF(TIME.LT.2.)GO TO 200
      IF(ATIME.LE.2.)GO TO 100
  200 WRITE(6,70)TIME,X1,X2,X1DEN,X2DEN,U,W
   70 FORMAT(1X,7E15.5)
      ATIME=0.
  100 CONTINUE
C***AIT1=COST ASSOCIATED WITH STATE
C***AIT2=COST ASSOCIATED WITH CONTROL
      AIT1=D(1,1)*(X1**2)+(D(1,2)+D(2,1))*X1*X2+D(2,2)*(X2**2)
      AIT2=R(1,1)*(U1**2)+(R(1,2)+R(2,1))*U1*U2+R(2,2)*(U2**2)
      SAIT=AIT1+AIT2
      AIT=AIT+(SAIT*DT)
      AITD =D(1,1)*(X1DEN**2)+(D(1,2)+D(2,1))*X1DEN*X2DEN+D(2,2)*(X2D
     1EN**2)
      AITDP=AITDP+AITD*DT
    1 CONTINUE
      COSTOP=.5*AITDP
      COST=.5*AIT
      WRITE(6,10)COST,COSTOP
   10 FORMAT(1X,//2E15.8)
      RETURN
      END
C
```

```
C
      SUBROUTINE PROC(C,COST)
C
C    THIS SUBROUTINE IS CALLED BY THE SEARCH TECHNIQUE TO EVALUATE THE
C    VALUE OF THE PERFORMANCE INDEX --- OPTION IS ALSO AVAILABLE TO
C    GENERATE AND PRINT OUT RESPONSE OF THE NONLINEAR SYSTEM
C
      COMMON VOL,DEN,DELH,CP,AKO,AKS,DS,DT,FTIME,X10,X20,Z,AKO,TFS,CFS,TO
     2UTS,COUTS,A,B,C,D,BINV,RK,N,NP,IA,AT,BT,PROD2,JOPT
      DIMENSION BINV(2,2),D(2,2),A(2,2),AT(2,2),B(2,2),BT(2,2),RK(2,2),A
     1A(2,2),P(2,2),PROD1(2,2),PROD2(2,2),PROD3(2,2),PROD4(2,2),PROD5(2
     2,2),PROD6(2,2),SUM(2,2),X(2,2),BINV1(2,2),C(10),STEP(10)
      TIME=0.
      IF(JOPT.EQ.0)GO TO 6
      WRITE(6,22)
   22 FORMAT(1X,33HRESPONSE WITH SEARCHED PARAMETERS)
    6 CONTINUE
      ITER=(FTIME/DT)+.5
      A=0.
      V=0.
      TF=0.
      CF=0.
      AIT=0.
      X1S=TOUTS
      X2S=COUTS
      X1=X10-.10
      X2=X20-.20
      DO 1 I=1,ITER
      FACTOR=(V+AKS)/(VOL*DEN)
      AK=AKO*(EXP(-Z/(X1+.60)))
      F1=FACTOR*(TF+TFS-X1-X1S)+((Q+QS)/(VOL*DEN*CP))-((DELH*(AK+AKS)*((
     1X2+.5)**2))/(DEN*CP))
      F2=FACTOR*(CF+CFS-X2-X2S)-(AK+AKS)*((X2+X2S)**2)
      IF(JOPT.EQ.0)GO TO 5
    5 CONTINUE
```

```
      TIME=TIME+DT
      X1=X1+(A1*DT)
      X2=X2+(A2*DT)
      U1=C(1)*X1          +C(2)*X2
      U2=C(3)*X1          +C(4)*X2
      U=U1
      V=U2
C***AIT1=COST ASSOCIATED WITH STATE
C***AIT2=COST ASSOCIATED WITH CONTROL
      AIT1=R(1,1)*(X1**2)+(R(1,2)+R(2,1))*X1*X2+R(2,2)*(X2**2)
      AIT2=R(1,1)*(U1**2)+(R(1,2)+R(2,1))*U1*U2+R(2,2)*(U2**2)
      SAIT=AIT1+AIT2
      AIT=AIT+(SAIT*DT)
    1 CONTINUE
      COST=.5*AIT
      IF(UNIT.EQ.0)GO TO 7
      WRITE(6,30)COST
   30 FORMAT(1X,//5HCOST=,F15.4)
    7 CONTINUE
      RETURN
      END
```

APPENDIX D

COMPUTER PROGRAMS FOR CHAPTER V

```
C
C
C   HYBRID PROGRAM FOR FEEDBACK CONTROL OF SIMPLE NONLINEAR SYSTEM
C
      DIMENSION          U(100)
      LOGICAL TRSL
C   LOGICAL VARIABLE TRSL CONTROLS TIMING --- FROM ANALOG CLOCK
      DATA U/100*0./
C   SUBROUTINE SPLIT SETS DAC BITS --FIRST NUMBER IS BIT NO.,SECOND
C   IS SETTING
      CALL SPLIT(00,.01)
      CALL SPLIT(01,.01)
      CALL SPLIT(02,.005)
      CALL SPLIT(03,.5)
      CALL SPLIT(73,.04)
C   ISAM IS COUNTER FOR SAMPLING
   99 ISAM=0
C   INITIALIZING CONTROL
      U0= .4*U
C   SUBROUTINE ITOA TRANSFERS VALUES BACK TO ANALOG
      CALL ITOA(2,U0)
   98 IF(.NOT.TRSL(2))GO TO 98
  100 ICT=0
C   CHECK SENSE SWITCH -- USED TO TERMINATE PROGRAM
      CALL SSWTCH(1,KSEN)
      IF(KSEN.LE.1)CALL RELEASE
    1 IF(.NOT.TRSL(2))GO TO 99
      IF(.NOT.TRSL(3))GO TO 1
C   SAMPLE VALUE OF STATE VARIABLE
      CALL CDAC(3,X)
C   SUBROUTINE CDAC READS VALUE OF ANALOG-DIGITAL CONVERTER
      X=X*10.
      ISAM=ISAM+1
C   PROGRAM DIRECTED TO POLYNOMIAL CORRESPONDING TO PROPER SAMPLING PT.
      GO TO (1,2,3,4,5),ISAM
```

```
C     LAMBDA VS X POLYNOMIALS FOLLOW
      2 ALA=.9951
        ICT=8
        GO TO 7
      3 ALA=.26079+.14309*X-.02924*X**2+.00212*X**3
        GO TO 7
      4 ALA=.17414+.28478*X-.07703*X**2+.00733*X**3
        GO TO 7
      5 ALA=.0117+.31412*X-.10121*X**2+.01281*X**3
        GO TO 7
      6 ALA=.01135+.18475*X-.04374*X**2+.00437*X**3
C
      7 X=X/10.
C     STATE AND CONTROL (OR LAMBDA) SENT BACK TO ANALOG AS INITIAL COND.
        CALL LTSA(0,X)
        CALL LTSA(1,ALA)
        I=0
     20 IF(.NOT.TRSL(1))GOTO20
        I=I+1
     21 IF(TRSL(1))GOTO21
        IF(I.LT.2)GO TO 20
C     SUBROUTINE SSCL SETS SENSE-LINE 0 --THIS IS USED TO START FAST
C     INTEGRATION THAT DETERMINES CONTROL UNTIL NEXT SAMPLING POINT
        CALL SSCL(0)
        I=0
      8 IF(.NOT.TRSL(1))GO TO 8
        I=I+1
        CALL CSAC(1,U)
C     VALUE OF CONTROL IS SAMPLED AND STORED IN ARRAY U
        U(I)=U
      9 IF(.NOT.TRSL(1))GO TO 10
        GO TO 9
     10 IF(I.LT. 50) GO TO 8
C     SUBROUTINE SSCL RESETS SENSE-LINE 0 -- THIS STOPS INTEGRATION
        CALL SSCL(0)
```

```
   13 ICT=ICT+1
      UD=U(ICT)
C    OPTIMAL CONTROL ARRAY, UD, IS TRANSFERED BACK TO ANALOG
C    IN REAL TIME TO CONTROL SYSTEM UNTIL NEXT SAMPLING POINT
      CALL LTLA(2,UD)
   11 IF(.NOT.TRSL(0))GO TO 12
      GO TO 11
   12 IF(.NOT.TRSL(2))GO TO 99
      IF(.NOT.TRSL(0))GO TO 12
      IF(ICT.LT.50)GO TO 13
      GO TO 100
      STOP
      END
```

```
C
C
C     HYBRID PROGRAM FOR APPROXIMATE OPTIMAL FEEDBACK CONTROL OF
C     CONTINUOUS STIRRED TANK REACTOR
C
        DIMENSION U(100),ATEST(100)
        LOGICAL TEST
        DATA U/100*0./,ATEST/100*0./
C
C     HYBRID SUBROUTINES ARE THE SAME AS DEFINED IN PREVIOUS EXAMPLE
C
C     SET PARTS
        CALL SPART(119,.3667)
        CALL SPART( 28,.0667)
        CALL SPART(52,.256)
        CALL SPART(47,.500)
        CALL SPART(20,.0014)
        CALL SPART(95,.0003)
        CALL SPART(37,.4)
        CALL SPART(97,.2)
        CALL SPART(50,.2744)
        CALL SPART(51,.0127)
        CALL SPART(72,.0004)
        CALL SPART(0,.0006)
        CALL SPART(45,.0667)
        CALL SPART(02,.2667)
        CALL SPART(40,.410)
        CALL SPART(10,.610)
        CALL SPART(41,.0667)
        CALL SPART(1,.0667)
        CALL SPART(63,.51)
        CALL SPART(3,.99)
        CALL SPART(67,.2560)
        CALL SPART(17,.2560)
        CALL SPART(71,.0274)
```

```
      CALL SPOT(25,.04)
      CALL SPOT(1,.2139)
      CALL SPOT(21,.2)
      CALL SPOT(25,.2)
      CALL SPOT(7,.2139)
      CALL SPOT(7,.61)
      CALL SPOT(25,.61)
C     ISAM IS SAMPLE NUMBER
   29 ISAM=0
      U0=-.12
C     TRANSFER INITIAL VALUE OF CONTROL
      CALL XTLA(5,J5)
C     LOGICAL VARIABLES TASL CONTROL TIMING FROM ANALOG CLOCK
   98 IF(.NOT.TASL(2))GO TO 98
  100 ICT=0
      CALL SAMPLE(1,KSEL)
      IF(KSEL.EQ.1)CALL RELEASE
    1 IF(.NOT.TASL(2))GO TO 99
      IF(.NOT.TASL(3))GO TO 1
C     SAMPLE CONCENTRATION,C, AND TEMPERATURE,T
      CALL GVAC(0,C)
      CALL GVAC(1,T)
C     MULTIPLY BY SCALE FACTORS
      T=T*1000.
      C=C*10.
      ISAM=ISAM+1
      GO TO (2,3,4,5,6),ISAM
    2 AL1=4.507
      AL2=1.38
      ICT=2
      GO TO 7
C     POLYNOMIALS BASED ON REGRESSION OF OFF-LINE SOLUTIONS FOLLOW
    3 AL1=294.51+1.*3.9*C-2.2737*C*T
      AL2=4.33+.7 +216.02*C-1.58*C**2-.0004*T**2-.1772*C*T
      GO TO 7
```

```
    4 AL1=10.96+1702.71*C-1.953*C*T
      AL2=134.31+151.35*C-.124*C*T
      GO TO 7
    5 AL1=74.  2+1123.1*C+14.825*C**2-1.2871*C*T
      AL2=-111.15+105.37*C+.2145*T-.1047*C*T
      GO TO 7
    6 AL1=450.14+161.94*C+21.192*C**2-.0017*T**3
      AL2=24.300+1.461*C-.0197*T+1.385*C**2
C   CALCULATE VALUE OF RATE CONSTANT,AKO,CORRESPONDING TO SAMPLED TEMP.
C   TO BE USED AS INITIAL COND. FOR IMPLICIT GENERATION OF K
    7 AKO=1.415*EXP(-2540./T)*10.
      T=T/1000.
      C=C/10.
      AL1=AL1/10000.
      AL2=AL2/10000.
C   TRANSFER BACK TO ANALOG VALUE OF T,C,LAMBDA1,LAMBDA2 AND RATE CONST.
      CALL LTDA(0,C)
      CALL LTDA(1,T)
      CALL LTDA(3,AL1)
      CALL LTDA(4,AL2)
      CALL LTDA(2,AKO)
      I=0
   20 IF(.NOT.TPSL(1))GO TO 20
      I=I+1
   21 IF(TPSL(1))GO TO 21
      IF(I.LT.20)GO TO 20
C   START FAST INTEGRATION
      CALL SSCL(0)
      I=0
    8 IF(.NOT.TPSL(1))GO TO 8
      I=I+1
      CALL GRAC(2,JD)
C   SAMPLE VALUE OF OPTIMAL CONTROL FROM FAST INTEGRATION AND STORE
C   IN ARRAY U
      U(I)=JD
```

```
    9 IF(.NOT.TPSL(1))GO TO 10
      GO TO 4
   10 IF(I.LT.50)GO TO 9
C    STOP FAST INTEGRATION
      CALL ISEL(0)
   13 ICT=ICT+1
      JD=J(ICT)
C    TRANSFER CONTROL,JD,BACK TO ANALOG TO CONTROL REACTOR
      CALL LTRA(5,JD)
   11 IF(.NOT.TPSL(4))GO TO 12
      GO TO 11
   12 IF(.NOT.TPSL(2))GO TO 99
      IF(.NOT.TPSL(3))GO TO 12
      IF(ICT.LT.50)GO TO 13
      GO TO 100
      STOP
      END
```

Vita

The author was born in New Orleans, Louisiana on February 21, 1944. He received his elementary school training at Metairie Junior High in Metairie, Louisiana; he graduated from De LaSalle High School in New Orleans, Louisiana in 1962.

In September of 1962 he entered the Louisiana State University at Baton Rouge from which he was graduated in August of 1966 with the Bachelor of Science degree in Chemical Engineering and in May of 1968 with the Master of Science degree in Chemical Engineering.

He was then employed in the Systems Engineering Department of the Louisiana Division of the Dow Chemical Company until June of 1969. He then entered the Graduate School of the Louisiana State University at Baton Rouge.

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EXAMINATION AND THESIS REPORT

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